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AFML-TR-65-2
Part IV, Volume III

TERNARY PHASE EQUILIBRIA IN TRANSITION METAL-
BORON-CARBON-SILICON SYSTEMS

Part IV. Thermochemical Calculations

Volume III. Computational Approach to the
Calculation of Ternary Phase
Diagrams

Y. A. Chang
Aerojet-General Corporation

TECHNICAL REPORT NO. AFML-TR-65-2, PART IV, VOLUME III.
October 1966

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Air Force Materials Laboratory
Research and Technology Division
Air Force Systems Command
Wright-Patterson Air Force Base, Ohio

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FOREWORD

The research described in this report was carried out at the Materials Research Laboratory, Aerojet-General Corporation, Sacramento, California, under USAF Contract No. AF 33(615)-1249. The contract was initiated under Project No. 7350, Task No. 753001, and was administered under the direction of the Air Force Materials Laboratory, Research and Technology Division, with Captain R. A. Peterson and Lt. P.J. Marchiando acting as Project Engineers, and Dr. E. Rudy, Aerojet-General Corporation, as Principal Investigator. Professor Dr. Hans Nowotny, University of Vienna, served as consultant to the program.

The project, which includes the experimental and theoretical investigation of related binary and ternary systems in the system classes Me_1-Me_2-C , $Me-B-C$, Me_1-Me_2-B , $Me-Si-B$, and $Me-Si-C$, was initiated on 1 January 1964. The work on related binary systems $Me-C$ and $Me-B$ was initiated November 1964 as a subtask to the investigation of the ternaries.

The author wishes to thank Dr. E. Rudy for his interest, advice and encouragement during the course of this work. He also wishes to thank J. Hwang for aspects of the mathematical analysis of the problem. The computer programs were prepared by Ray Marler, Len Nole, Jerry Howard, and Bill Reuss of the Computing Science Division.

The manuscript of this report was released by the author February 1966 for publication as an RTD Technical Report.

Other reports issued under USAF-Contract AF 33(615)-1249 have included:

Part I. Related Binaries

Volume I.	Mo-C System
Volume II.	Ti-C and Zr-C Systems
Volume III.	Systems Mo-B and W-B
Volume IV.	Hf-C System
Volume V.	Ta-C System. Partial Investigations in the Systems V-C and Nb-C
Volume VI.	W-C System. Supplemental Information on the Mo-C System
Volume VII.	Ti-B System
Volume VIII.	Zr-B System
Volume IX.	Hf-B System
Volume X.	V-B, Nb-B, and Ta-B Systems

Part II. Ternary Systems

Volume I.	Ta-Hf-C System
Volume II.	Ti-Ta-C System
Volume III.	Zr-Ta-C System

FOREWORD (Cont'd)

- Volume IV. Ti-Zr-C, Ti-Hf-C, and Zr-Hf-C Systems
- Volume V. Ti-Hf-B System
- Volume VI. Zr-Hf-B System
- Volume VII. Ti-Si-C, Nb-Si-C and W-Si-C Systems
- Volume VIII. Ta-W-C System
- Volume IX. Zr-W-B System, Pseudobinary System TaB₂-HfB₂
- Volume X. Zr-Si-C, Hf-Si-C, Zr-Si-B, and Hf-Si-B Systems
- Volume XI. Hf-Mo-B and Hf-W-B Systems

Part III. Special Experimental Techniques

- Volume I. High Temperature Differential Thermal Analysis

Part IV. Thermochemical Calculations

- Volume I. Thermodynamic Properties of Group IV, V, and VI Transition Metal Carbides
- Volume II. Thermodynamic Interpretation of Ternary Phase Diagrams.

This technical report has been reviewed and is approved.



W.G. RAMKE
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ABSTRACT

The general conditional equations which govern the phase equilibria in three-component systems are presented. Using the general conditional equations, a general method has been developed to precalculate the phase equilibria in three-component systems from first principle using computer technique. The method developed has been applied to several model examples and the system Ta-Hf-C. The phase equilibria in three-component systems calculated using the simplified method as originally developed by Rudy, agree well with those calculated by the present method. The only difference is in the homogeneous range with respect to the interstitial component of solid solutions which exhibit large variation with metal exchange. This is to be expected in view of the assumptions made in the simplified method.

In connection with the phase diagram calculation and other problems of the present Air Force contract, several computer programs have been developed which are included in the appendix of this report.

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I. INTRODUCTION AND SUMMARY

A. INTRODUCTION

Apart from theoretical interest, the capability of predicting phase equilibria in three-component systems from binary data is of practical significance since the cost of experimentally investigating phase equilibria in ternary systems is rather high. For the transition metal₁, metal₂-carbon ternary systems (i.e. the interstitial type of solid solutions), a method has been developed by Rudy⁽¹⁾ to predict the phase equilibria in ternary systems assuming that the intermediate phases in the metal₁-carbon and metal₂-carbon binaries are either of line-compounds or that both phases are of equal dependence of the free energy on the concentration coordinate of the interstitial component. In cases, where the homogeneous ranges of the solid solutions with respect to the interstitial component changes drastically with metal exchange, the simplified method does not predict, as to be expected from the assumptions made, the exact phase boundaries. The purpose of the present work is to develop a general method using computer technique to predict the phase equilibria in three-component systems with no assumptions made as in the simplified method. This general method will predict not only the phase equilibria but also the correct homogeneous ranges of the single phases.

B. SUMMARY

The conditional equations which govern the phase equilibria in three-component systems are presented. Using the conditional equations, a method has been developed using computer technique to precalculate the phase equilibria in three-component systems from first principle. The method developed has been applied to model examples and the system Ta-Hf-C. The phase equilibria in three-component systems calculated using the simplified method originally developed by Rudy, agree rather well with those calculated by the present method. The only difference is in the homogeneous ranges of solid solutions which exhibit large variation with metal exchange. This is to be expected in view of the assumptions made in the simplified method.

Several computer programs for the phase equilibrium calculations as well as for other problems of the present Air Force contract have been developed. The fortran statements of all the computer programs are included in the appendix at the end of the report.

II. THERMODYNAMIC DESCRIPTION OF PHASE EQUILIBRIA IN THREE COMPONENT SYSTEMS

According to the phase rule, at constant pressure the maximum number of coexisting phases in a one-component system is two, two-component system three, and three-component system, four. In addition, if one fixes temperature, the maximum number of coexisting phases in a ternary system reduces to three. Consequently, an isothermal section of a ternary phase diagram is built up of one-phase, two-phase, and three-phase equilibria. On the one hand, concentrations of the coexisting phases in a two-phase field determine the phase boundaries of single-phase fields. On the other hand, the boundaries of a three-phase equilibrium are the limiting tie-lines of the three adjacent two-phase equilibria. We shall now discuss first the thermodynamics of two-phase equilibria.

A. TWO-PHASE EQUILIBRIA IN THREE-COMPONENT SYSTEM

The Gibbs free energy of formation of a two-phase alloy, $A_x B_y C_z$ as shown in Figure 1 is a linear combination of the Gibbs free energies of formation of the two coexisting phases $A_x' B_y' C_z'$ and $A_{x''} B_{y''} C_{z''}$. Expressing in mathematical terms, we have

$$\Delta G = \nu_1 \Delta G_1 + \nu_2 \Delta G_2 \quad (1)$$

where ΔG , ΔG_1 , and ΔG_2 are the Gibbs free energies of formation of the two-phase alloy and of the two co-existing single phases; and ν_1 and ν_2 are the relative amounts of the two co-existing single phases. If we take one gramatom of alloy as our basis, we have the following three boundary conditions:

$$v_1 + v_2 = 1 \quad (2)$$

$$x' + y' + z' = 1 \quad (3)$$

$$x'' + y'' + z'' = 1 \quad (4)$$

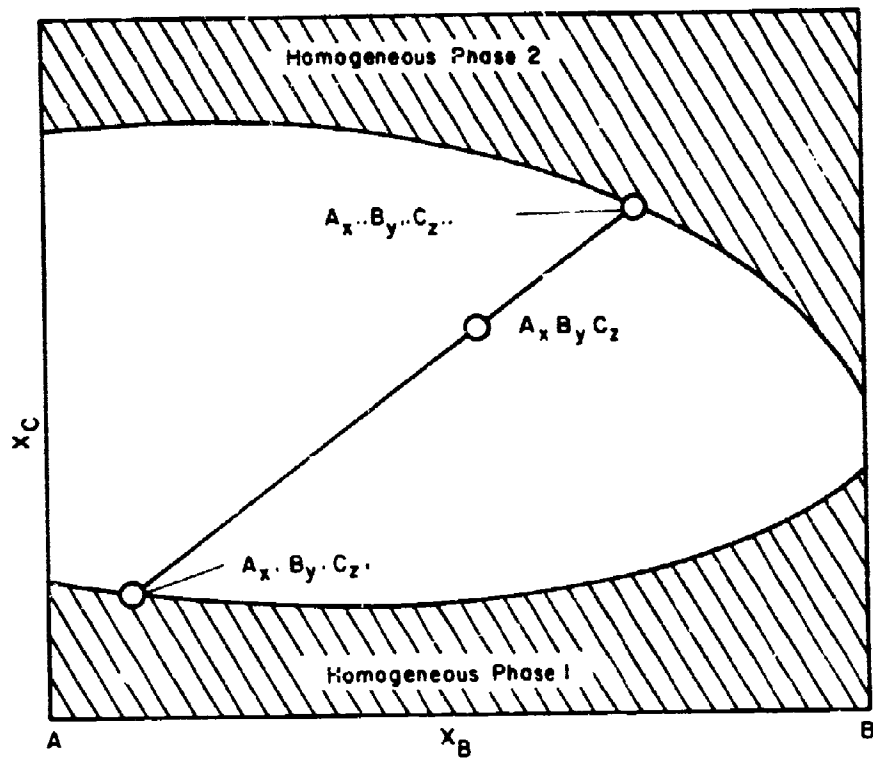


Figure 1. Two-Phase Equilibria in a Ternary System.

Two additional boundary conditions can be obtained resulting from the conservation of masses:

$$v_1 x' + v_2 x'' = x \quad (5)$$

$$v_1 y' + v_2 y'' = y \quad (6)$$

Given ΔG_1 and ΔG_2 as a function of composition at constant P and T and a set of x, y, z values, we would like to calculate the values of x', y', z' and $x'', y'',$ and z'' . Since there are eight unknowns: $v_1, v_2, x', y', z', x'', y'',$ and z'' and five equations (2 to 6), we have only three independent variables. We can choose any three variables as we wish. In the present case, we shall choose $x', y',$ and x'' , as our ultimate variables. By elimination of the various variables in equations (2) through (6), we obtain the following expressions for v_1, v_2, z', y'' and z'' in terms of x', y' and x'' :

$$v_1 = \frac{x - x''}{x' - x''} \quad (7)$$

$$v_2 = \frac{x - x'}{x'' - x'} \quad (8)$$

$$z' = 1 - x' - y' \quad (3a)$$

$$y'' = \frac{x' - x''}{x' - x} y + \frac{x - x''}{x - x'} y' \quad (9)$$

and

$$z'' = 1 - x'' - y'' \quad (4a)$$

In order to solve for x', y' and x'' , we need three additional equations which must be derived from the condition that at equilibrium ΔG according to equation (1) is a minimum. We can minimize ΔG , with the five constraints expressed by equations (2) through (6), after the method of Lagrange as was originally done by Rudy⁽¹⁾. We obtain,

$$\Delta G_1 - a_1 \quad -a_4 x' \quad -a_5 y' = 0 \quad (10)$$

$$\Delta G_2 - a_1 \quad -a_4 x'' \quad -a_5 y'' = 0 \quad (11)$$

$$v_1 \frac{\partial \Delta G_1}{\partial x'} - a_2 \quad -a_4 v_1 = 0 \quad (12)$$

$$v_1 \frac{\partial \Delta G_1}{\partial y'} - a_2 \quad -a_5 v_1 = 0 \quad (13)$$

$$v_1 \frac{\partial \Delta G_1}{\partial z'} - a_2 = 0 \quad (14)$$

$$v_2 \frac{\partial \Delta G_2}{\partial x''} - a_3 - a_4 v_2 = 0 \quad (15)$$

$$v_2 \frac{\partial \Delta G_2}{\partial y''} - a_3 - a_5 v_2 = 0 \quad (16)$$

$$v_2 \frac{\partial \Delta G_2}{\partial z''} - a_3 = 0 \quad (17)$$

From equations (12), (13), (15), and (16); (12), (14), (15), and (17); and (12), (14), (15), and (17), we obtain the following additional equations:

$$\left[\frac{\partial \Delta G_1}{\partial x'} - \frac{\partial \Delta G_1}{\partial y'} \right]_{T,p} = \left[\frac{\partial \Delta G_2}{\partial x''} - \frac{\partial \Delta G_2}{\partial y''} \right]_{T,p} \quad (18)$$

$$\left[\frac{\partial \Delta G_1}{\partial z'} - \frac{\partial \Delta G_1}{\partial x'} \right]_{T,p} = \left[\frac{\partial \Delta G_2}{\partial z''} - \frac{\partial \Delta G_2}{\partial x''} \right]_{T,p} \quad (19)$$

and

$$\Delta G_1 - \Delta G_2 = (x' - x'') \left[\frac{\partial \Delta G_1}{\partial x'} - \frac{\partial \Delta G_1}{\partial z'} \right]_{T,p} + (y' - y'') \left[\frac{\partial \Delta G_1}{\partial y'} - \frac{\partial \Delta G_1}{\partial z'} \right]_{T,p} \quad (20)$$

From equations (18), (19), and (20), we can in principle solve for x'' , x' , and y' . However, since the equations for ΔG_1 and ΔG_2 are non-linear with respect to the three independent variables x'' , x' , and y' , the solving of the three simultaneous equations is not very simple. Instead, it is more convenient to numerically find the minimum value of ΔG according to equation (1) by varying the values of x'' , x' , and y' from 0.0 to 1.0. We can take any small incremental value as we wish. In general, for phase diagram calculations, we have found a value of 0.01 is sufficient.

Since $x' + y' \leq 1$, we need only to consider the values of x' , y' , and x'' in the prism as shown in Figure 2 for the computation of ΔG . Moreover

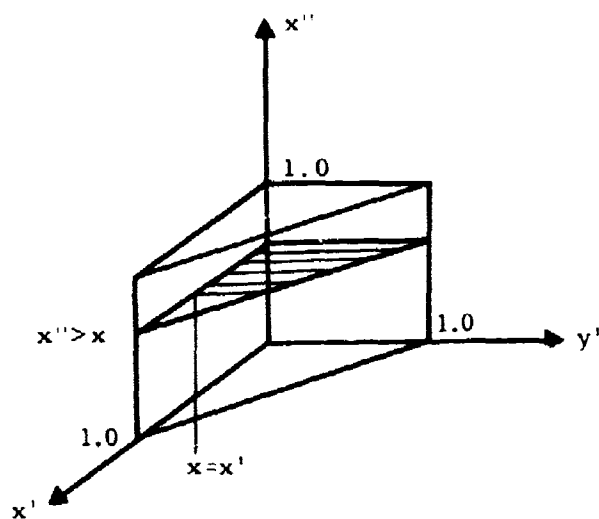


Figure 2. Schematic Representation of the Three Independent Variables x' , y' and x'' for Two-Phase Equilibria in a Ternary System when $x'' > x$.

the values of x always lie between those of x' and x'' . For each value of x'' greater than x , we compute ΔG for all values of x' smaller than x , i.e. the shaded trapezoidal region (in Figure 2) and for each value of x' smaller than x , we do the similar computations for all values of x' greater than x , i.e. the shaded trapezoidal region in Figure 3.

Since v_1, v_2 and y'' are all positive, rearranging equation (6), we have

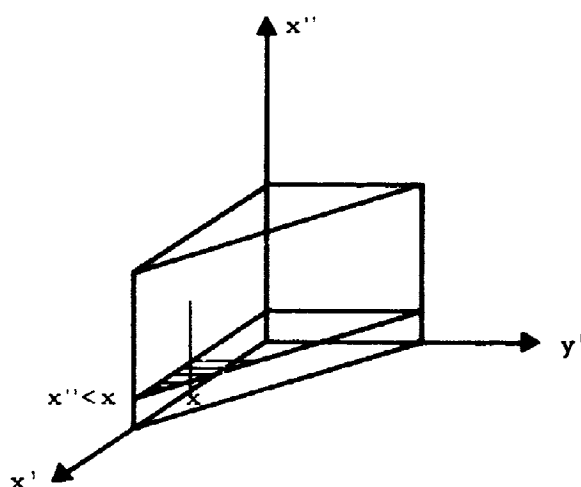


Figure 3. Schematic Representation of the Three Independent Variables x' , y' , and x'' for Two-Phase Equilibria in a Ternary System when $x'' < x$

$$y' = \frac{y}{v_1} - \frac{v_2}{v_1} y'' \leq \frac{y}{v_1} = \frac{x' - x''}{x - x''} y \quad (21)$$

Equation (21) gives an upper limit of y' .

The number of computations for searching the minimum of ΔG according to equation (1) can be further reduced when we use the additional information provided by the binary phase boundaries.

Before proceeding further, we must have some mathematical expressions for ΔG_1 and ΔG_2 . As shown previously,^(2,3) the free energy of a

single phase of the interstitial type of solid solutions such as the ternary
~~carbides may be adequately represented by the following expression,~~
 may be adequately represented by the following expression,

$$\Delta G_1 \text{ (in cal/gatom alloy)} = x' \Delta G_{AC_u} + y' \Delta G_{BC_u} + \frac{x'y' \epsilon'}{(1-z')} + RT \left[x' \ln \frac{x'}{1-z'} + y' \ln \frac{y'}{1-z'} \right] \quad (22)$$

where x' , y' and z' are atom fractions of A, B, and C in phase 1, ϵ' is the interaction parameter for the solid solution $(A,B)C_u$, R is the universal gas constant, T is the absolute temperature, and ΔG_{AC_u} and ΔG_{BC_u} are the Gibbs free energies of formation of the two respective binary phases in cal/gatom A or B. We have a similar expression for ΔG_2 which is a function of x'' , y'' and z'' .

Often we have the cases where the solubility of the third component, let's say C, in the solution $(A,B)C_u$ is so small that for practical purposes, we can take u as zero. For such cases, $z' = 0$, we reduce the three independent variables x' , y' and z' to only x' and x'' . Therefore, the search for a minimum for ΔG according to equation (1) reduces from a three-dimensional to a two-dimensional problem.

Model Example 1:

Let us now take a hypothetical case where A and B form a series of continuous solid solutions at high temperature; A and C and B and C form two intermediate phases AC_v , AC_w and BC_v , BC_w , respectively as shown in Figures 4 and 5. Moreover, the solubility of C in the solid solution (A,B) is assumed to be small; and $(A,B)C_v$ and $(A,B)C_w$ form two series of continuous solid solutions. The homogeneous range with respect to component C is narrow in the solid solution $(A,B)C_w$ solid solution. We would like now to compare the tie-line distributions in the two-phase regions $(A,B)-(A,B)C_v$ and $(A,B)-(A,B)C_w$ calculated at 2000°K using the method described here with those calculated by the simplified method⁽¹⁾.

The Gibbs free energies of the four binary intermediate phases: AC_v , BC_v , AC_w , and BC_w may be represented by the following equations (see Figures 4 and 5).

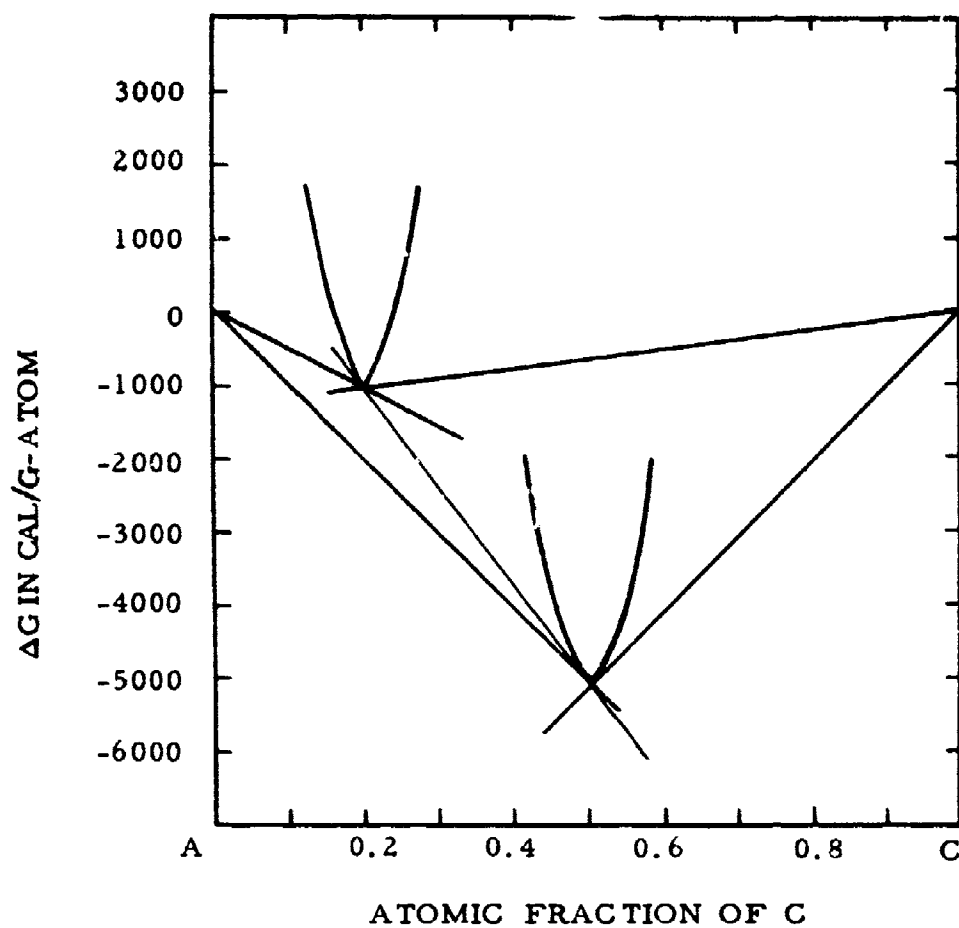


Figure 4. Gibbs Free Energies of the Two Intermediate Phases AC_v and AC_w in the binary A-C.

$$\Delta G_{AC_v} = \frac{1}{1-z} \{23,000 - 240,000 z + 600,000 z^2\} \quad (23)$$

$$\Delta G_{BC_v} = \frac{1}{1-z} \{35,710 - 418,882 z + 1,102,162 z^2\} \quad (24)$$

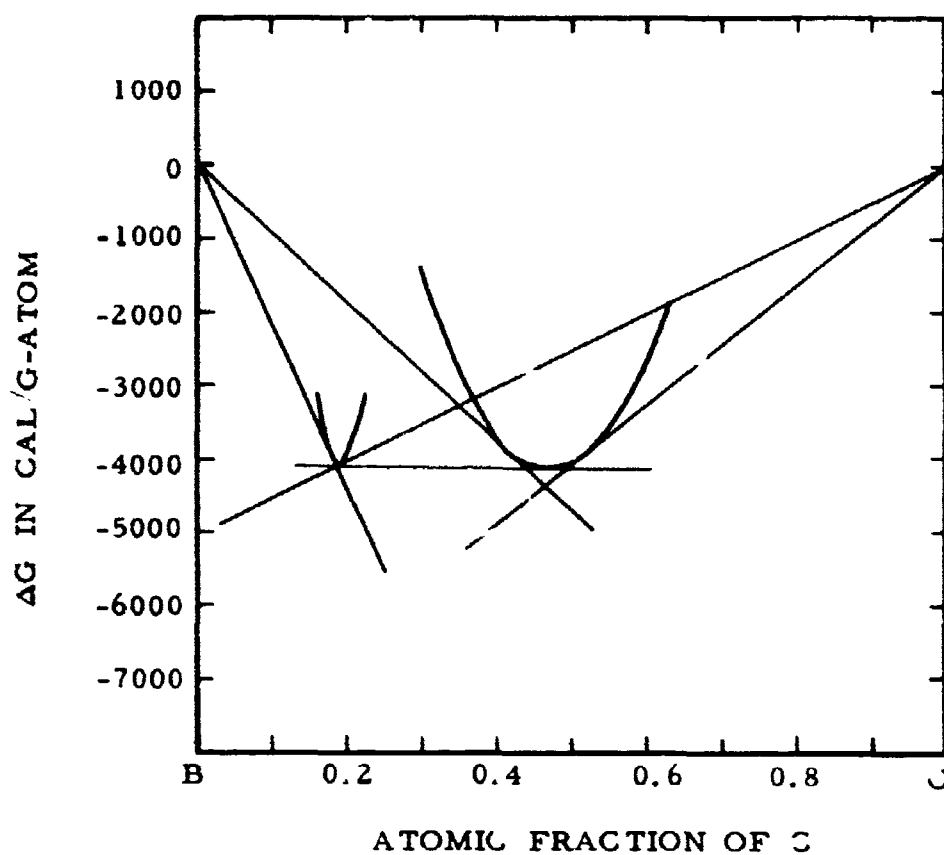


Figure 5. Gibbs Free Energies of the Two Intermediate Phases BC_v and BC_w in the Binary A-C.

$$\Delta G_{AC_w} = \frac{1}{1-z} \{121,065 - 504,220 z + 504,220 z^2\} \quad (25)$$

$$\Delta G_{BC_w} = \frac{1}{1-z} \{15,335 - 83,555 z + 89,780 z^2\} \quad (26)$$

The Gibbs free energies of the ternary solutions $(A,B)C_v$ and $(A,B)C_w$ may take the same form as equation (22). The interaction parameters for the three solid solutions are taken to be,

$${}^{\circ}A,B = 5970$$

$${}^{\circ}(A,B)C_v = 3980$$

$${}^{\circ}(A,B)C_w = 3980$$

We shall first consider the two-phase equilibria between the solid solutions (A,B) and (A,B)C_v. Since we assume that the intermediate phases AC_w and BC_w are not stable in the binary systems, the phase AC_v then becomes stable. Accordingly, we have

$$\Delta G_1 = 5970 x'y' + RT (x' \ln x' + y' \ln y') \quad (27)$$

$$\begin{aligned} \Delta G_2 = & x''\Delta G_{AC_v} + y''\Delta G_{BC_v} + \frac{3980 x''y''}{1-z''} + \\ & + RT \left[x'' \ln \frac{x''}{1-z''} + y'' \ln \frac{y''}{1-z''} \right] \end{aligned} \quad (28)$$

One can see from Figures 6 and 7 that the tie-line distribution between the solid solutions (A,B) and (A,B)C_v calculated using the method described here agrees well with that calculated using the simplified method. This is to be expected since the range of homogeneity with respect to component C in (A,B)C_v is relatively narrow. The simplified method for calculating the two-phase equilibria in ternary systems has been discussed extensively by Rudy⁽¹⁾. It suffices to say that the compositions of the two co-existing phases are where the concentration free energy gradients are the same, i.e.

$$\frac{d\Delta G_1}{dx'} = \frac{d\Delta G_2}{dx''} \quad (29)$$

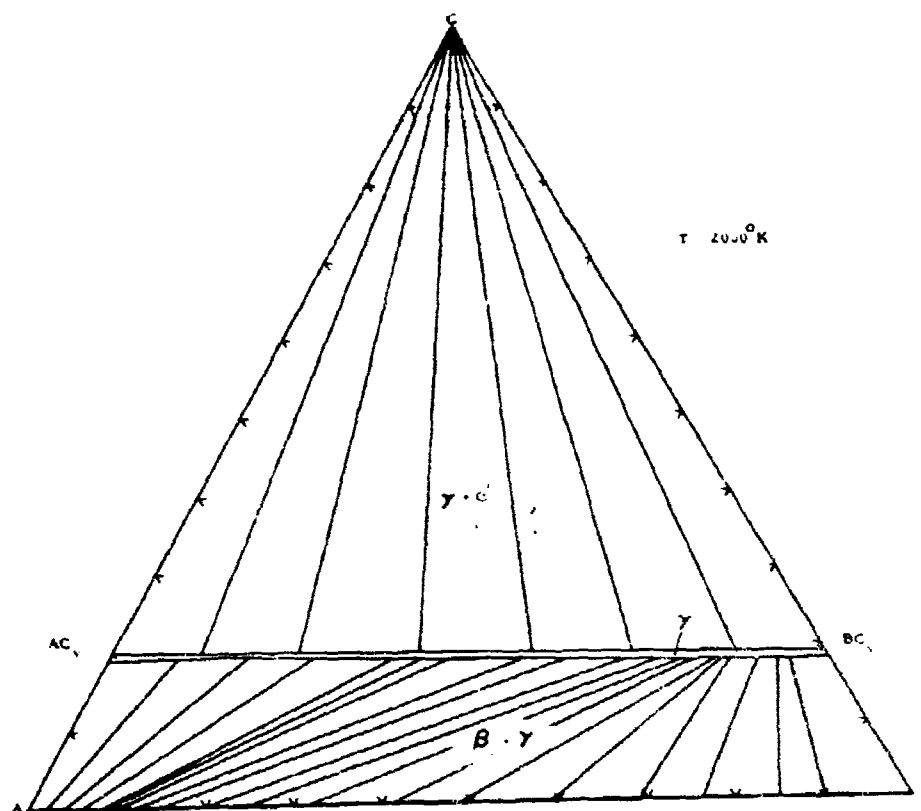


Figure 6. Phase Equilibria Between Phases β and γ and γ and C in the System A-B-C at 2000°K Calculated Using the General Method.

The concentration free energy gradient curves for the solid solutions (A,B), (A,B) C_v and (A,B) C_w are shown in Figure 8.

Next, we consider the two-phase equilibria between the solid solutions (A,B) and (A,B) C_w . In this case, we assume that the phases AC_v and BC_v do not appear in the two respective binaries. Since the homogeneous range for the phase BC_w is relatively large and the free energies of AC_w phase increase rapidly at concentrations of C-component higher and lower

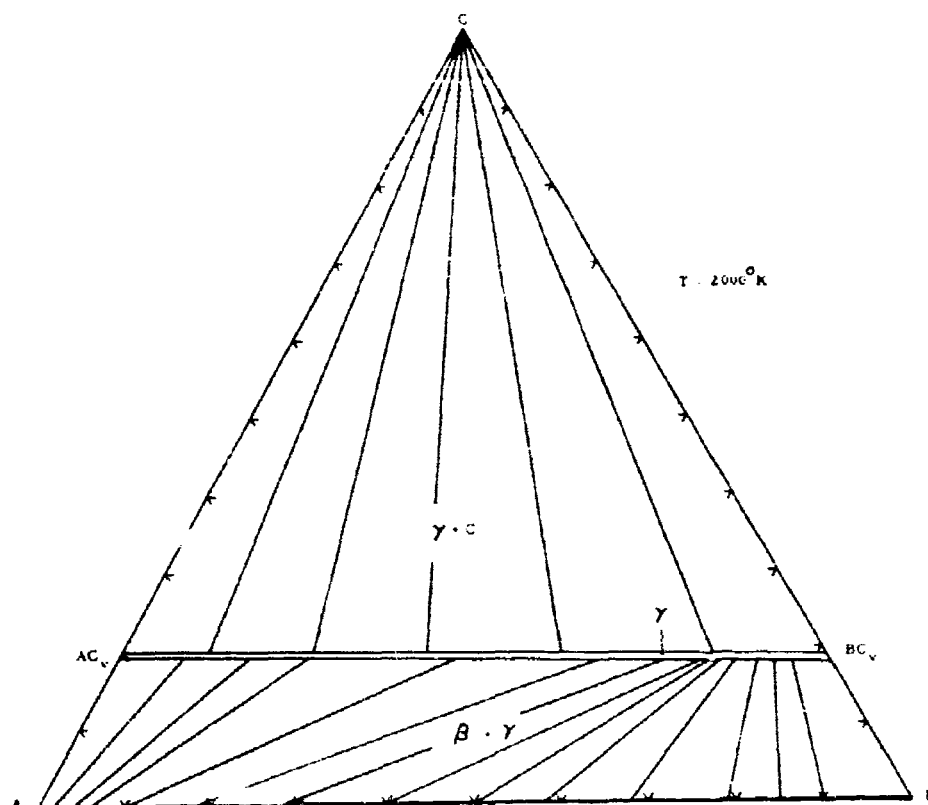


Figure 7. Phase Equilibria Between Phases β and γ and γ and C in the System A-B-C at 2000°K Calculated Using the Simplified Method.

0.5, the tie-line distribution calculated (Figure 9) used this simplified method does not agree well with that calculated (Figure 10) using the general method described here again as expected. Moreover, the A-B-rich phase boundary of the solid solution $(A,B)C_w$ calculated using the method described in this paper shows a curvature as expected while that calculated using the simplified method does not.

It should be pointed out here since the solubilities of A and B in C are assumed to be negligible, the tie lines in the two-phase regions $(A,B)C_v$ and C and $(A,B)C_w$ and C (Figures 6, 7, 9, and 10) were not calculated and must be pointed toward the pure component.

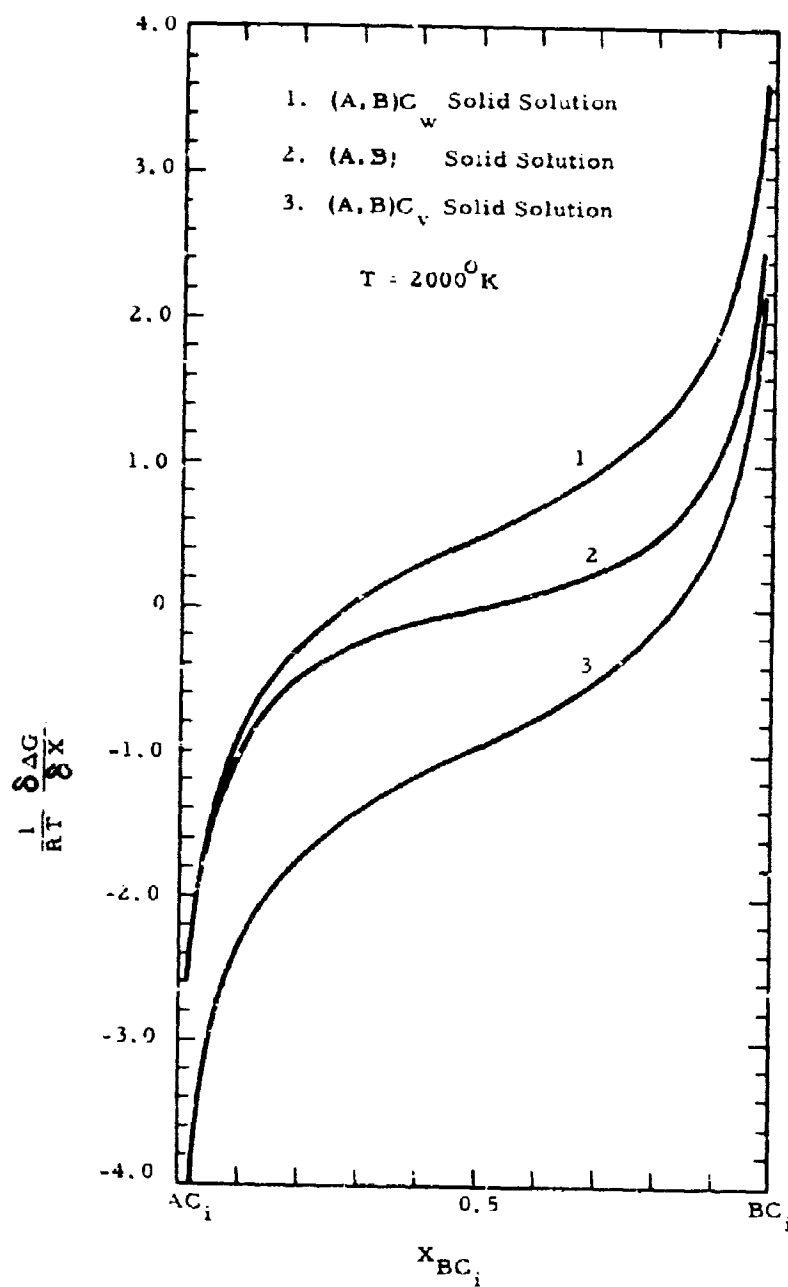


Figure 8. Concentration Free Energy Gradient Curves for Solutions (A,B) , $(A,B)C_v$ and $(A,B)C_w$ at 2000°K .

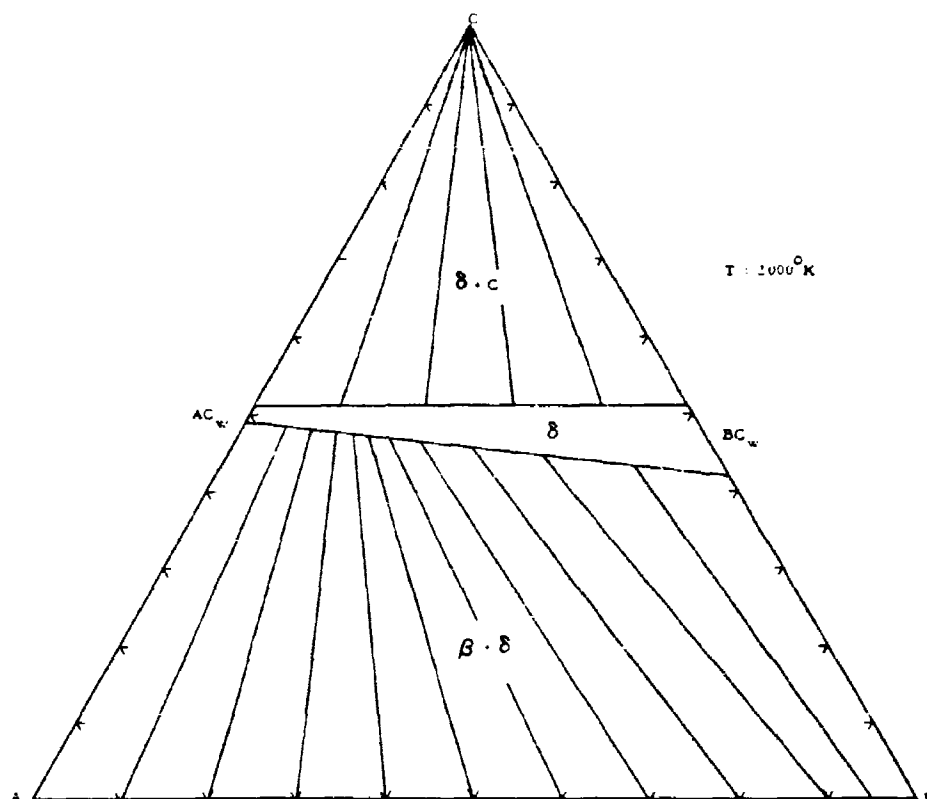


Figure 9. Phase Equilibria Between β and δ and δ and C in the System A-B-C at 2000°K Calculated Using the Simplified Method.

B. THREE-PHASE EQUILIBRIA IN THREE-COMPONENT SYSTEM

In a similar manner as for the two-phase equilibria, the Gibbs free energy of a three-phase alloy $A_x B_y C_z$ as shown in Figure 11 is a linear combination of the Gibbs free energies of formation of the three co-existing phases $A_{x'} B_{y'} C_{z'}$, $A_{x''} B_{y''} C_{z''}$ and $A_{x'''} B_{y'''} C_{z'''}$:

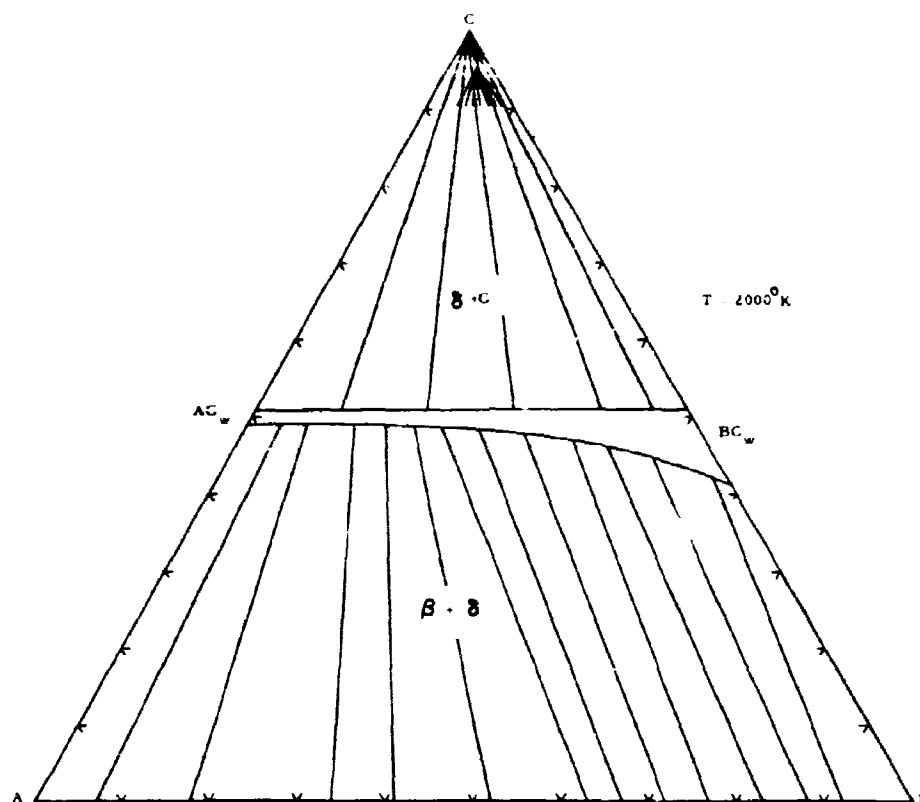


Figure 10. Phase Equilibria Between β and δ and δ and C in the System A-B-C at 2000°K Calculated Using the General Method.

$$\Delta G = \nu_1 \Delta G_1 + \nu_2 \Delta G_2 + \nu_3 \Delta G_3 \quad (30)$$

with the following constraints:

$$\nu_1 + \nu_2 + \nu_3 = 1 \quad (31)$$

$$x' + y' + z' = 1 \quad (32)$$

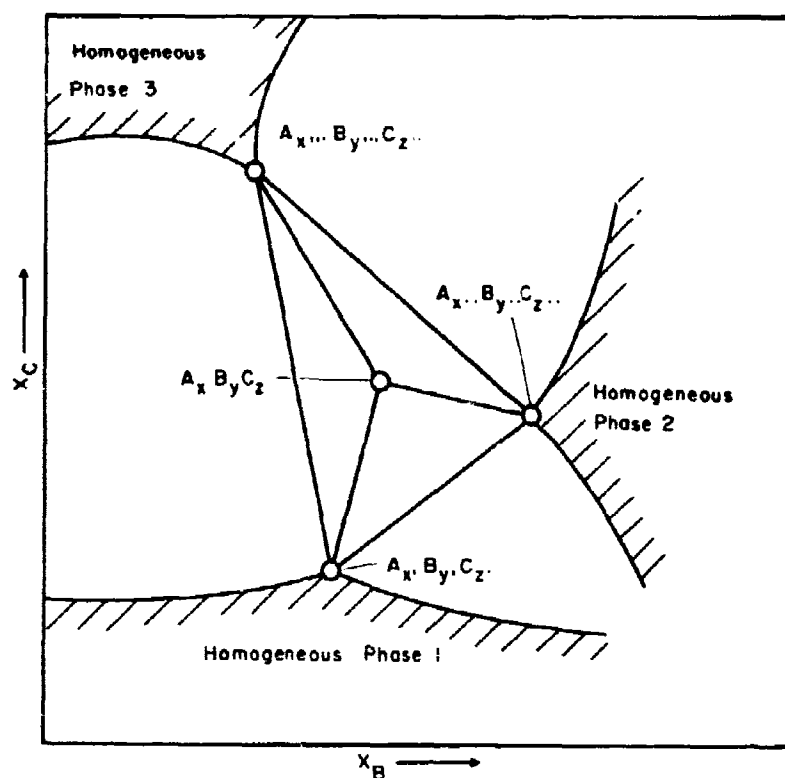


Figure 11. Three-Phase Equilibrium in a Ternary System

$$x'' + y'' + z'' = 1 \quad (33)$$

$$x''' + y''' + z''' = 1 \quad (34)$$

$$v_1 x' + v_2 x'' + v_3 x''' = x \quad (35)$$

$$v_1 y' + v_2 y'' + v_3 y''' = y \quad (36)$$

We have twelve unknowns and six equations (31 through 36). Therefore, we have six independent variables. It is no longer practical for us to use the similar method as for the two-phase equilibria to find the combination of the compositions of the three co-existing phases where ΔG according to equation (30) is a minimum.

Fortunately, we can reduce the six independent variables to two by taking advantage of the fact that the boundaries of a three-phase equilibrium are nothing but the limiting tie-lines of the three adjacent two-phase equilibria. We shall first discuss the method of seeking the compositions (x''' , y''' , z''') of the third co-existing phase when the compositions (x' , y' , z' and x'' , y'' , z'') of the other two co-existing phases are known. We will then discuss how to find the compositions x' , y' , z' and x'' , y'' , z'' . Under such conditions, instead of having the six constraints as expressed by equations (31) through (36), we have only four boundary conditions: Equations (31), (34), (35), and (36) with six unknowns, i.e. v_1 , v_2 , v_3 , x''' , y''' and z''' . Therefore, we have ultimately two independent variables. We can choose any two variables as we wish, but from a practical point of view, it is convenient to choose the two variables z''' and y''' . Expressing v_1 , v_2 , v_3 and x''' in terms of y''' and z''' ; we have

$$v_1 = \frac{(y' - y)(z''' - z) - (z'' - z)(y''' - y)}{D} \quad (37)$$

$$v_2 = \frac{(y - y')(z''' - z') - (z - z')(y''' - y')}{D} \quad (38)$$

$$v_3 = 1 - v_1 - v_2 \quad (31a)$$

$$x''' = 1 - y''' - z''' \quad (34a)$$

where

$$D = (y'' - y')(z''' - z') - (z' - z')(y''' - y') \quad (39)$$

To find the values of y''' and z''' we again have to use the condition that at equilibrium ΔG according to equation (30) is a minimum. The method for seeking the values of y''' and z''' where ΔG is a minimum is similar to the method used for solving the two-phase equilibria discussed earlier.

For the three-phase equilibria resulting from a miscibility gap in one of the solid solutions, the compositions of the miscibility gap of this solid solution are well-defined. In this case, we can solve for the composition of third co-existing phase using the method described here.

Model Example 2.

We shall use the same data as in Model Example 1 to illustrate the application of the method described here. When the temperature is lower from 2000°K to 1250°K, a miscibility gap results from the solid solution (A, B). The compositions of the miscibility gap at 1250°K are $x' = 0.83$, $y' = 0.17$ and $x'' = 0.17$ and $y'' = 0.83$. Again, as shown in Figures 12 and 13, the phase equilibria calculated using the simplified method agree well with those calculated using the general method with the exception that homogeneous range of the solid solution (A, B)C_v with respect to component C is narrower. The free energy-concentration-gradient curves used to determine the phase equilibria at 1250°K as shown in Figure 12, are displaced in Figure 14.

Referring to Figure 15, the method for seeking the composition of the three co-existing phases β - γ - δ will be discussed using the following conditions:

$$\begin{array}{lll}
 \text{at } x_1, y_1, z_1: & \Delta G (2\phi \text{ between } \beta-\delta) & < \Delta G(2\phi \text{ between } \beta-\gamma) \\
 & & < \Delta G(3\phi \text{ between } \beta-\gamma-\delta) \\
 \\
 \text{at } x_2, y_2, z_2: & \Delta G (3\phi \text{ between } \beta-\delta-\gamma) & < \Delta G(2\phi \text{ between } \beta-\delta) \\
 & & < \Delta G(2\phi \text{ between } \beta-\gamma) \\
 \\
 \text{at } x_3, y_3, z_3: & \Delta G (2\phi \text{ between } \beta-\gamma) & < \Delta G(2\phi \text{ between } \beta-\delta) \\
 & & < \Delta G(3\phi \text{ between } \beta-\gamma-\delta)
 \end{array}$$

In reality, we don't have any idea about the compositions of the three co-existing phases except we know there is a three-phase equilibrium β - γ - δ since the corresponding phase in the A-C binary is not stable. Thus, we can start, let's say, with a composition x_1, y_1, z_1 and ask ourselves what possible three-phase field it is in. We know one of the phase boundaries of this three-phase equilibrium β - γ - δ is the tie-line between β - δ and furthermore, this tie-line must lie at the left of the composition x_1, y_1, z_1 . Thus, we can start with various compositions at the left of the composition x_1, y_1, z_1 and first find the corresponding compositions of the two co-existing phases β and δ . Knowing the various values of x', y', z' (β -phase) and x'', y'', z'' (δ -phase), one can calculate the corresponding values of x''', y''', z''' (γ -phase) and the corresponding values of $\Delta G (3\phi \text{ between } \beta-\delta-\gamma)$. One then compares the lowest value among all the ΔG values calculated with those of $\Delta G (2\phi \text{ between } \beta-\delta)$ and $\Delta G(2\phi \text{ between } \beta-\gamma)$

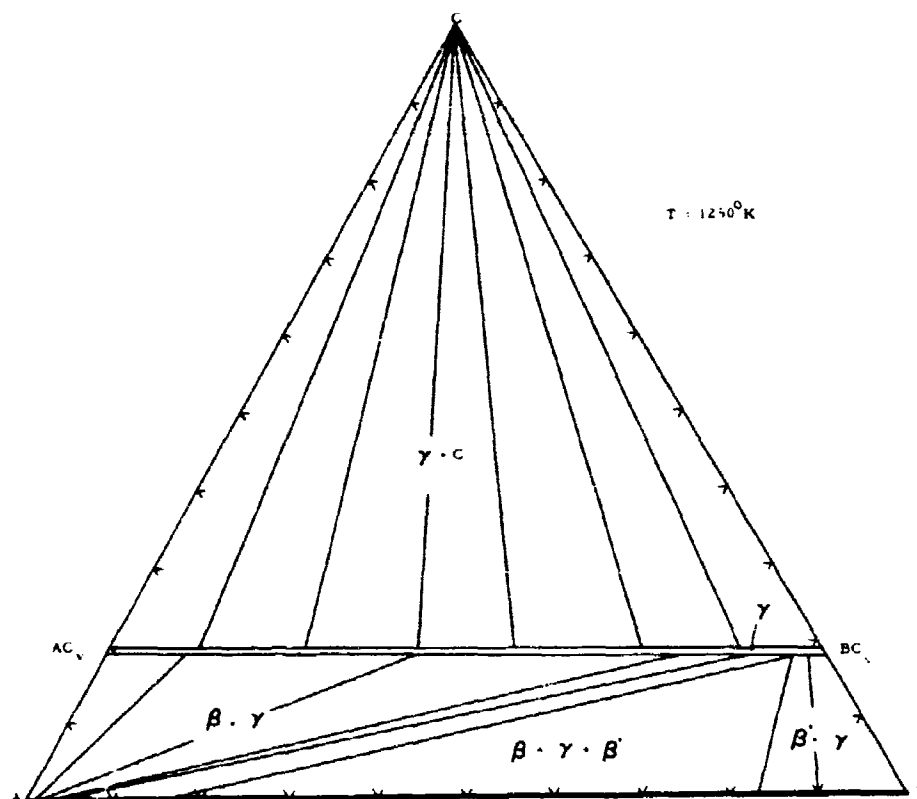


Figure 12. The Phase Equilibria Calculated Using the Simplified Method in the System A-B-C at 1251°K When the Two Binary Phases AC_w and BC_w are Unstable.

using the method described earlier. The stable equilibrium is defined by the lowest value of the Gibbs free energy. If ΔG (2 ϕ between β - δ) is the lowest, the three-phase equilibrium must lie at the right of the chosen values of x_1, y_1, z_1 . If on the other hand, the value of ΔG (2 ϕ between β - γ) is the lowest, then the three-phase equilibrium must lie to the left of the chosen values of x_1, y_1, z_1 . If the value of ΔG (3 ϕ between β - γ - δ) is the lowest, then we have found the three-phase equilibrium. A simple and rapid iteration process can be prepared to solve the compositions of the three co-existing phases.

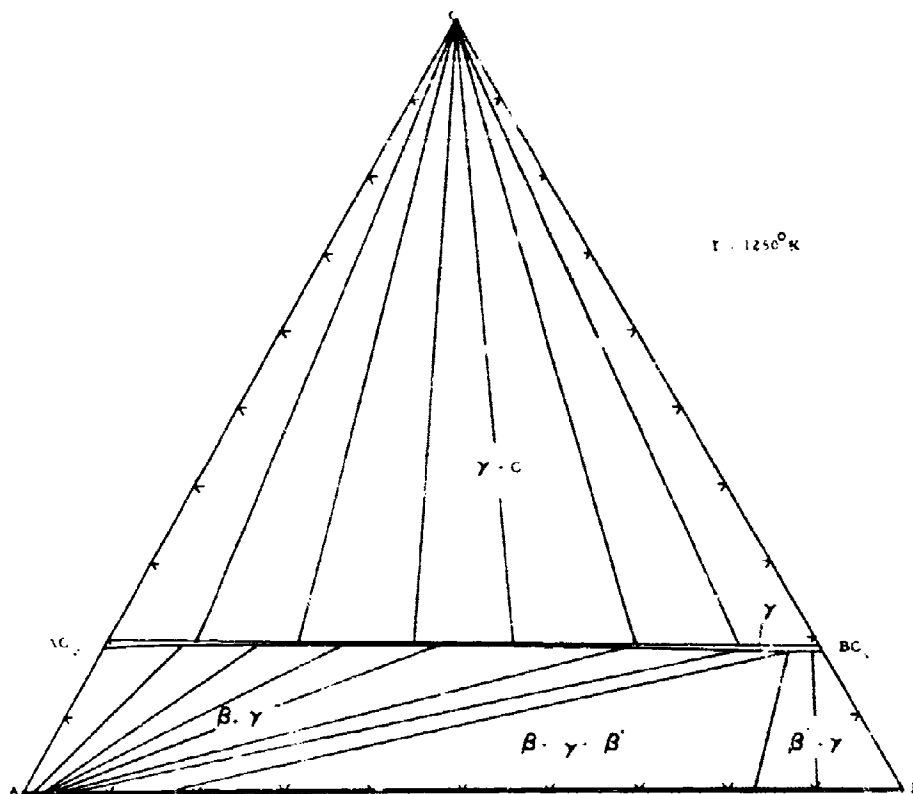


Figure 13. The Phase Equilibria Calculated Using the General Method in the System A-B-C at 1250°K When the Two Intermediate Phases AC_w and BC_w are Unstable.

Model Example 3:

Using the same data as in Model Example 1 and assuming all the three phase BC_v , AC_w and BC_w appear in the corresponding two binaries A-C and B-C, we shall use the method described here to find the three-phase field $\beta-\gamma-\delta$ and the tie-lines in the three two-phase fields: $\beta-\delta$, $\beta-\gamma$ and $\gamma-\delta$. The phase diagrams calculated at 2000°K using the general method as shown in Figure 16 agrees well with that calculated using the simplified method (Figure 17). The obvious difference between the two calculated

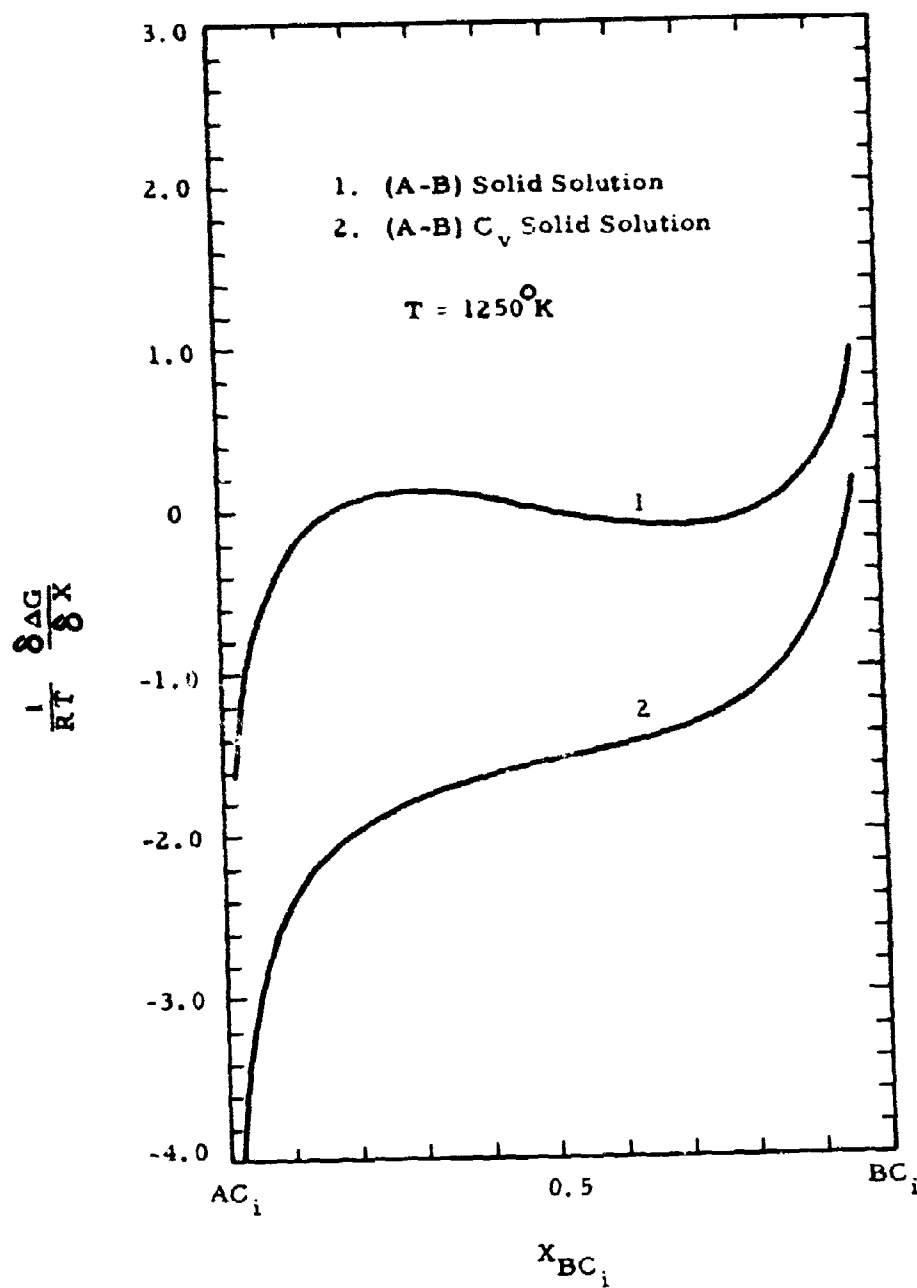


Figure 14. The Concentration-Free-Energy-Gradient Curves for Solutions (A,B) and (A,B) C_v at 1250°K.

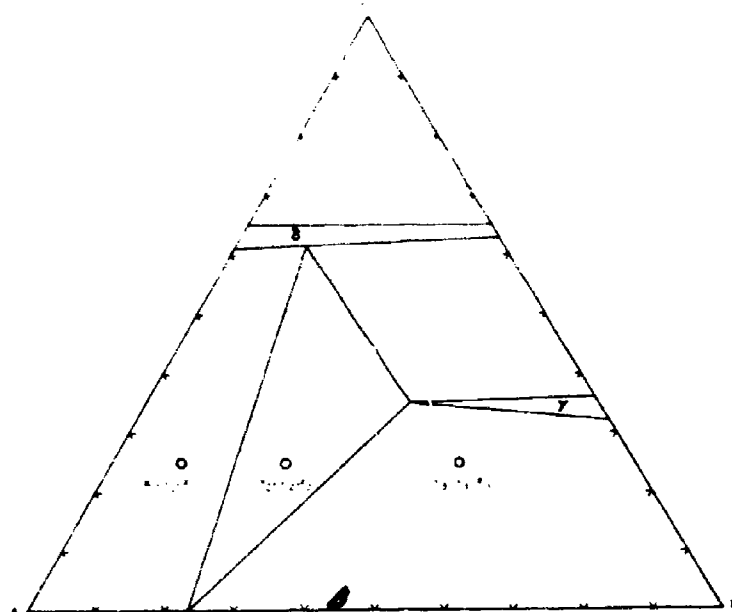


Figure 15. A Typical Ternary Phase Diagram with a Three-Phase Field Resulting from the Absence of a Corresponding Intermediate Phase in the Binary A-C.

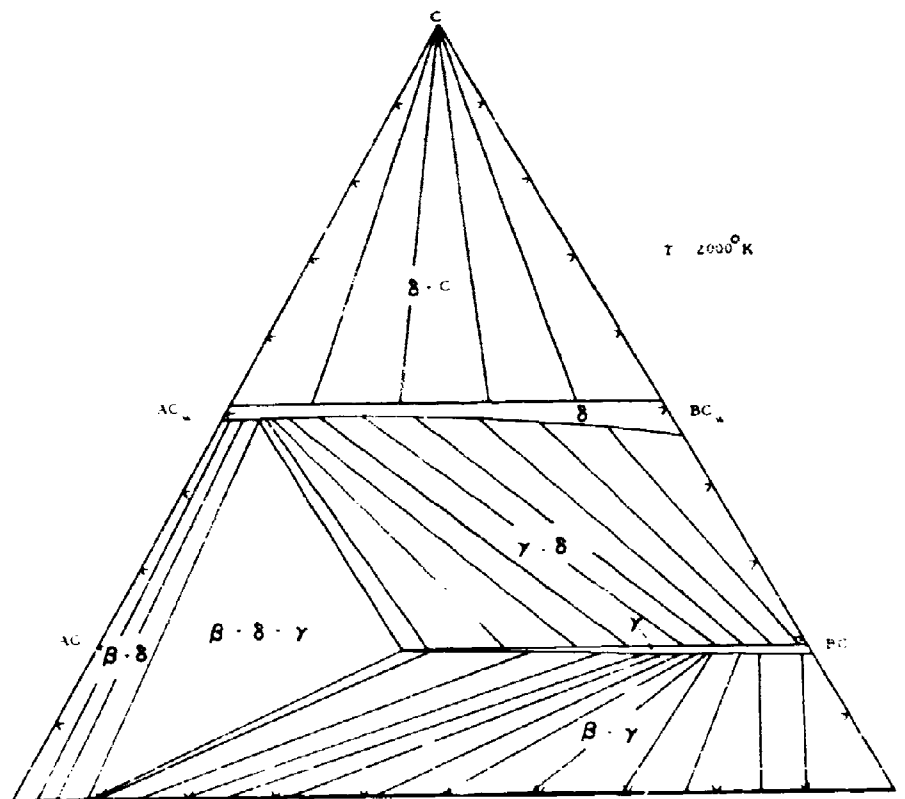


Figure 16. Phase Equilibria Calculated Using the General Method in the System A-B-C at 2000°C when the three Phases AC_w , BC_v and BC_w are Stable in the Binaries

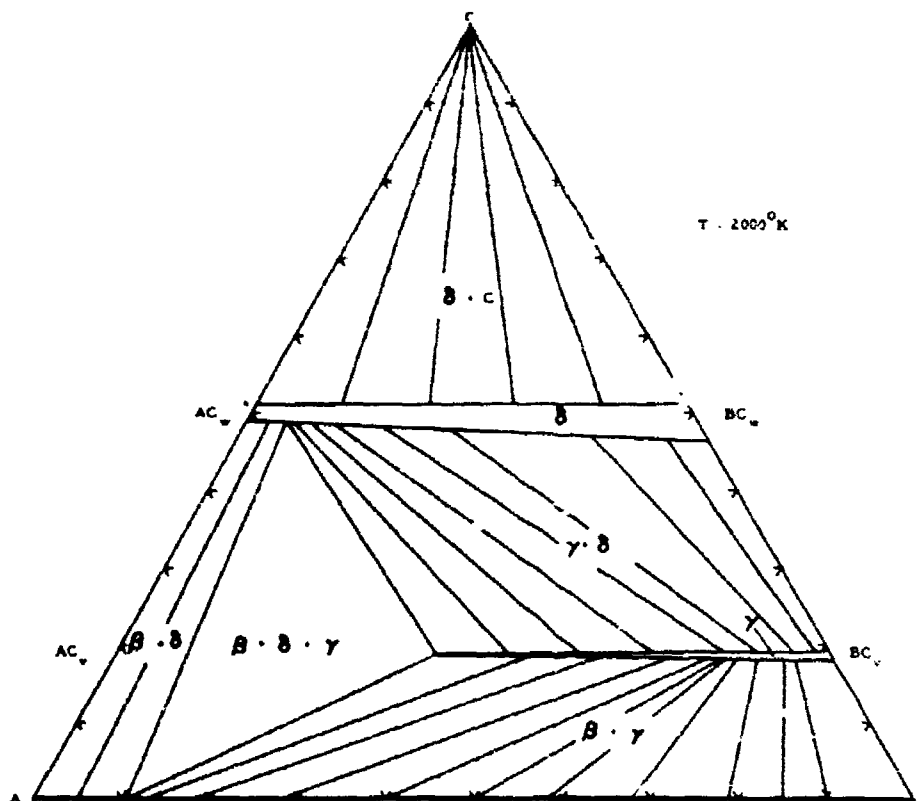


Figure 17. Phase Equilibria Calculated Using the Simplified Method in the System A-B-C at 2000°K When the Three Phases AC_w , BC_v and BC_w are Stable in the Binaries.

phase diagrams is the (A-B) rich homogeneous range of the solid solution (A-B) C_w with respect to C-component. The homogeneous range calculated using the general method shows the curvature while that calculated using the simplified method does not.

Although the technique of fixing the compositions of the co-existing phases for a three-phase equilibrium using the simplified method has been discussed extensively previously, it is worthwhile to point out that in addition to the condition at equilibrium, the free-energy-concentration gradients, i.e.

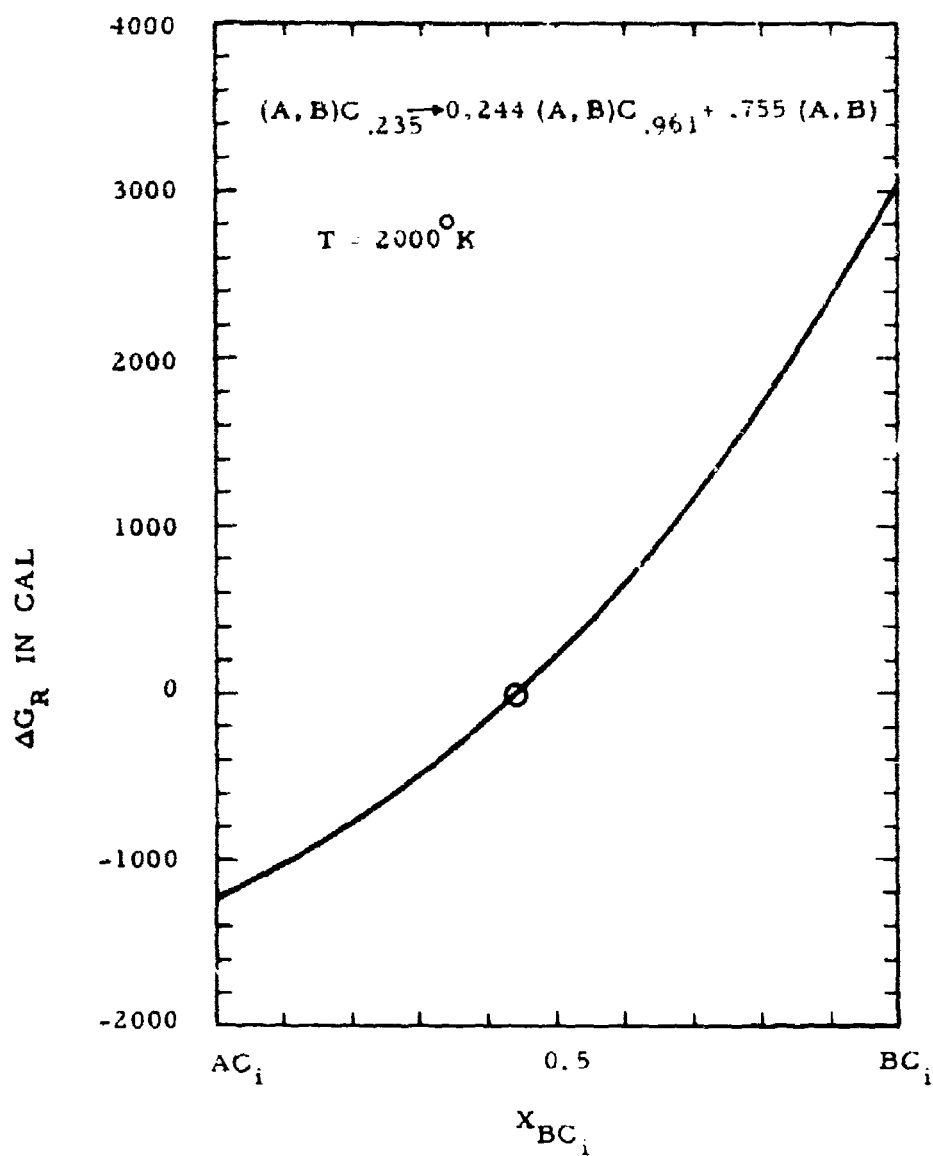
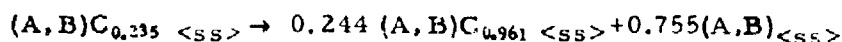


Figure 18. Integral Gibbs Free Energies of Decomposition of $(A,B)C_{.235}$ to $(A,B)C_{.961}$ and (A,B) .

$$\frac{\partial \Delta G_{(A,B)C_i}}{\partial x_{BC_i}}$$

must all be necessarily equal, we need the additional stability condition in order to fix the compositions of the three phases. Expressing in thermodynamic terms, the stability condition simply says that at equilibrium the integral Gibbs free energy of decomposing an alloy $(A,B)C_v$ into two other alloys $(A,B)C_u$ and $(A,B)C_w$ must be zero. For the model example described here, the total Gibbs free energy of decomposition of the alloy $(A,B)C_{0.235}$ to the alloys $(A,B)C_{0.961}$ and (A,B) according to the following reaction is shown in Figure 18.



III. APPLICATION OF THE METHOD DEVELOPED TO THE SYSTEM Ta-Hf-C

As already discussed earlier, in order to precalculate the phase equilibria in a ternary system, it is necessary to know the free energies of the binary phases as a function of composition and the solution behaviors of the ternary phases. In the binary system Hf-C, one intermediate phase, hafnium monocarbide HfC (B1-type), forms with a wide range of homogeneity⁽⁴⁾. The α -Hf terminal phase is stabilized by the addition of carbon atoms to higher temperatures. However, since little is known about the free energy of this phase as a function of composition, we shall at the present ignore the stabilization of the α -phase to high temperatures and assume that metal and carbon components at the metal-rich boundaries of the monocarbide phase are in equilibrium with those in the β -Hf terminal phase at high temperatures.

In addition to the monocarbide phase (B1-type), a second intermediate phase, Ta_2C forms in the system tantalum-carbon. Tantalum subcarbide, Ta_2C , is polymorphic. The low-temperature form, α - Ta_2C , has a hexagonal close-packed arrangement of the metal atoms. The distribution of the carbon atoms among the interstitial sites is not known but undoubtedly dependent on temperature.

The high-temperature form β -Ta₂C, probably has the same arrangement of metal atoms⁽⁵⁾ but differs in the degree of disorder in the carbon sublattice from the α -modification. Again, for the lack of pertinent thermodynamic data with respect to the two modifications of Ta₂C, we shall assume α -Ta₂C and β -Ta₂C to be of one phase for the calculation at the present.

The Gibbs free energies of the monocarbide and subcarbide phases will be represented by a sum of two contributions: the thermal and the configurational contributions to the total free energies of these phases, i.e.

$$\Delta G = \Delta G^{\text{th}} + \Delta G^{\text{conf}} \quad (39)$$

Since the free energies of formation⁽⁶⁾ for both of the two monocarbide phases at the stoichiometric composition have been determined, we shall represent the free energies of formation due to thermal vibration for compositions less than $x_C = 0.5$ by,

$$\Delta G^{\text{th}} (\text{B1 phase}) = 2(1-z) \Delta G_f + (1-2z)(a + bz + Cz^2) \quad (40)$$

where ΔG_f is the Gibbs free energy of formation of the stoichiometric monocarbide phase in cal/gatom alloy, z is the atom fraction of the carbon component, and a , b and c are parameters needed to be determined. When b and c are set equal to zero, we have the Wagner-Schottky^(6, 7, 8, 9) vacancy model with 'a' being the Gibbs free energy of forming a carbon vacancy on the carbon sublattice. For the free energy contribution due to configurational mixing of carbon atoms among the various lattice sites, we assume ideal entropy of mixing which is reasonable at high temperatures. Accordingly, we have

$$\Delta G^{\text{conf}} = RT \left[z \ln \frac{z}{1-2z} + (1-z) \ln \frac{1-2z}{1-z} \right] \quad (41)$$

For the subcarbide phase, the thermal contribution to the total free energy will be represented by a 3rd degree polynomial, i.e.

$$\Delta G^{\text{th}} = a' + b'z + c'z^2 + d'z^3 \quad (40b)$$

For the configurational free energy, we shall use the model developed by Rudy⁽¹⁰⁾. In this model, one assumes that the two interstitial sites occupied by the carbon atoms are energetically different by an amount of ΔE . Expressing in terms of two gram atoms of metal (Me_2C_w), the configurational free energy as derived earlier⁽¹⁰⁾ is

$$\Delta G_{\text{Me}_2\text{C}_w}^{\text{conf}} = z_B \Delta E + \left[z_A \ln z_A + (1-z_A) \ln (1-z_A) + z_B \ln z_B + (1-z_B) \ln (1-z_B) \right] RT \quad (42)$$

where ΔE is the energy difference between the two interstitial sites in the cal/2-gram atom metal, z_A is the mole fraction of carbon atoms on the A-sites, $(1-z_A)$ is the mole fraction of vacant A-sites, z_B is the mole fraction of the carbon atoms on the energetically unfavorable B-sites and $(1-z_B)$ is the mole fraction of the vacant B-sites. It is understood that

$$z_A + z_B = w \quad (43)$$

However, since it is more convenient to discuss the free energies of solid solutions in terms of one gram atom alloy, we shall divide equation (42) by $(2+w)$ and change the variable from w to z (the atom fraction of carbon atoms in the solution). Accordingly, we have

$$\Delta G_{\text{Me}_{1-z}\text{C}_z}^{\text{conf}} = \frac{1-z}{2} \left[z_B \Delta E + \left[z_A \ln z_A + (1-z_A) \ln (1-z_A) + z_B \ln z_B + (1-z_B) \ln (1-z_B) \right] RT \right] \quad (44)$$

Using the well-known thermodynamic relationships relating the partial molar and integral quantities, we have,

$$\begin{aligned}
\Delta \bar{G}_{Me}^{conf} &= \Delta G - z \frac{d\Delta G}{dz} \\
&= \frac{z_B \Delta E}{2} + \frac{RT}{2} \left[z_A \ln z_A + (1-z_A) \ln (1-z_A) + \right. \\
&\quad \left. + z_B \ln z_B + (1-z_B) \ln (1-z_B) \right] \\
&\quad - \frac{z}{1-z} \left[\Delta E s + RT r \ln \frac{z_A}{1-z_A} + RT s \ln \frac{z_B}{1-z_B} \right]
\end{aligned}$$

$$\Delta \bar{G}_C^{conf} = \Delta G + (1-z) \frac{d\Delta G}{dz} \quad (45)$$

$$= \Delta E s + r RT \ln \frac{z_A}{1-z_A} + s RT \ln \frac{z_B}{1-z_B} \quad (46)$$

where

$$r = \frac{(1-z_A)^2 (1+u)^2}{(1-z_A)^2 (1+u)^2 + e^{-\Delta E/RT}} \quad (47)$$

$$s = \frac{(1-z_B)^2 (1+v)^2}{(1-z_A)^2 (1+u)^2 + e^{-\Delta E/RT}} \quad (48)$$

$$u = \frac{z_A}{1-z_A} e^{-\frac{\Delta E}{RT}} \quad (49)$$

$$v = \frac{z_B}{1-z_B} e^{\frac{\Delta E}{RT}} \quad (50)$$

$$\begin{aligned}
z_B = & \frac{-\left[\frac{1-3z}{1-z} + e^{-\frac{\Delta E}{RT}} \left(\frac{1+z}{1-z} \right) \right] + \left[\left(\frac{1-3z}{1-z} + e^{-\frac{\Delta E}{RT}} \frac{1+z}{1-z} \right)^2 + \left(\frac{8z}{1-z} \right) e^{-\frac{\Delta E}{RT}} \left(1 - e^{-\frac{\Delta E}{RT}} \right) \right]^{1/2}}{2(1 - e^{\Delta E/RT})} \quad (51)
\end{aligned}$$

$$z_A = \frac{2z}{1-z} - z_B \quad (52)$$

If we set $\Delta E = 0$, $z_A = z_B$ since there is no difference between the carbon atoms on the A-sites and B-sites. From equation (52) one obtains,

$$z_A = z_B = \frac{z}{1-z} \quad (53)$$

Substituting for z_A and z_B according to equation (53), equation (44) reduced to equation (41).

Before we can proceed any further, we must know the values of a, b, c , (equation 40a) and of a', b', c' (equation 40b) for the monocarbide and subcarbide phases in addition to the values of ΔE for the two subcarbide phases. These parameters were determined by using the following conditions.

- a. Values of ΔG_f for TaC and HfC are those selected by Chang⁽⁶⁾.
- b. The free energy decomposition of TaC_{0.5} to 0.633 TaC_{0.79} + 0.367 Ta is taken to be 2300 cal at 2273°K⁽⁶⁾.
- c. The free energy difference between HfC_{0.5} and TaC_{0.5} is taken to be 2250 cal at 2273°K⁽⁶⁾.
- d. The phase boundaries of the subcarbide and monocarbide phases are those determined by Rudy⁽⁴⁾ and Rudy and Harmon⁽⁵⁾.
- e. The partial molar quantities in the two-phase regions: metal-subcarbide, subcarbide-monocarbide and monocarbide-graphite must be all the same.

With these five conditions, we have obtained the following results for our computation:

HfC-phase (B1-type)

$$\begin{aligned} 2\Delta G_{f,0.5} &= -52,350 + 2.08 T & 298.15^\circ\text{--}2073^\circ\text{K} \\ &= -55,630 + 3.66 T & 2073^\circ\text{--}2491^\circ\text{K} \end{aligned}$$

$$a = 250,154; \quad b = -968,150; \quad c = 1,113,170$$

Hf₂C-phase

$$a' = 72,445; \quad b' = -466,000; \quad c' = 650,000; \quad d' = 0; \quad \Delta E = 0$$

TaC-phase (B1-type)

$$\begin{aligned} \Delta G_{f,0.5} &= -35,335 - 1.7949 \log T + 6.4757 T \\ a &= 363,950; \quad b = 1,527,083; \quad c = 1,770,833 \end{aligned}$$

Ta₂C-phase

$$\begin{aligned} a' &= 129,848; \quad b' = 1,336,117; \quad c' = -4,716,667; \quad d' = 5,373,333 \\ \Delta E &= 4000 \text{ cal.} \end{aligned}$$

The phase equilibria in the system Ta-Hf-C at 2273°K and 1273°K are calculated and presented in Figures 19 and 20. The phase diagrams calculated using the simplified method are shown in Figures 21 and 22 for comparison. As might be expected, the marked difference between the calculated phase diagrams by the two different methods is the homogeneous range of the monocarbide phase. The concentration-free-energy-gradient curves for the metal, subcarbide and monocarbide phases as well as the integral free energy of decomposition of the subcarbide phase into the metal and monocarbide phases at 2273°K used to establish the phase equilibria are presented in Figures 23 and 24. Similar curves used to determine the phase equilibria at 1773°K are not included in this report.

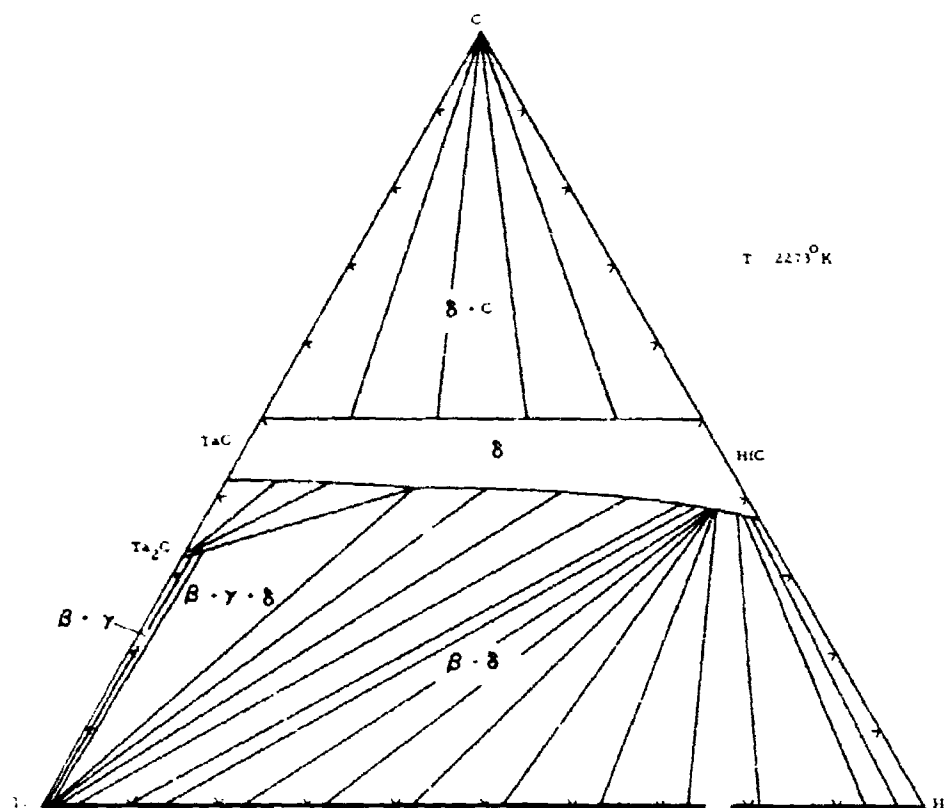


Figure 19. Calculated Phase Equilibria in the System Ta-Hf-C Using the General Method at 2273°K.

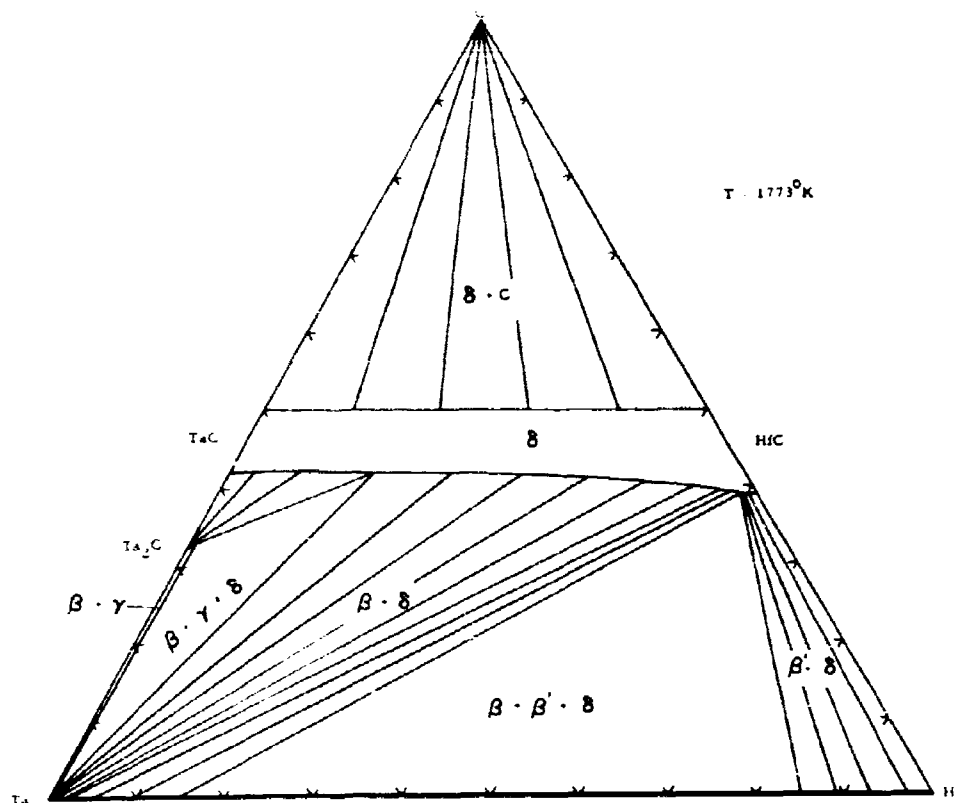


Figure 20. Calculated Phase Equilibria in the System Ta-Hf-C Using the General Method at 1773°K.

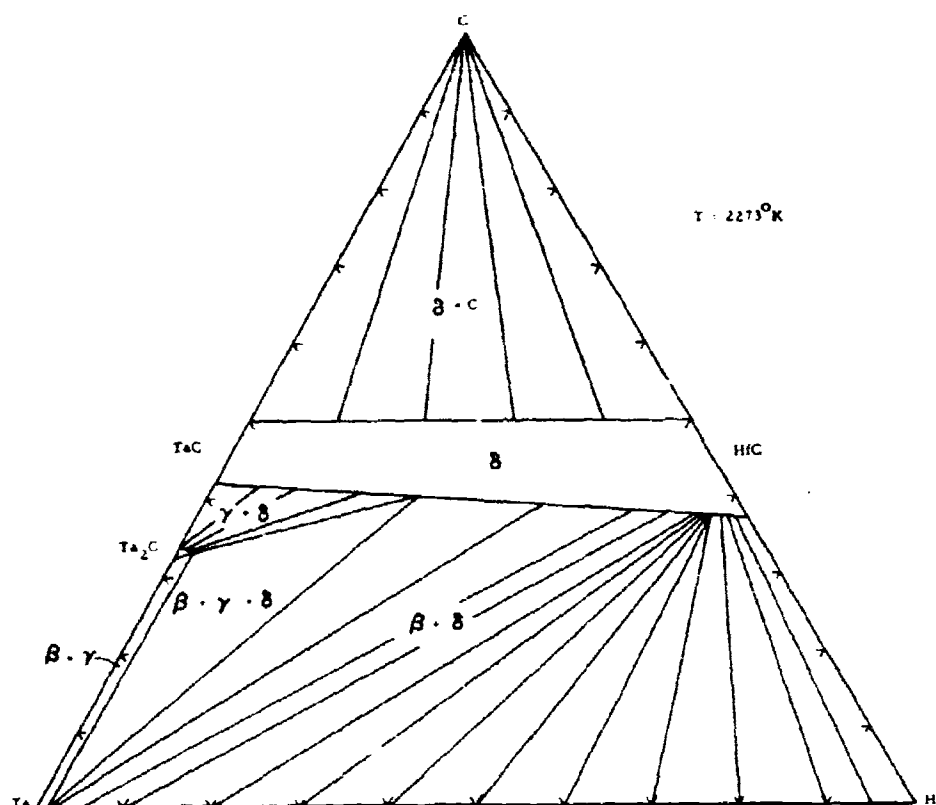


Figure 21. Calculated Phase Equilibria in the System Ta-Hf-C Using the Simplified Method at 2273°K.

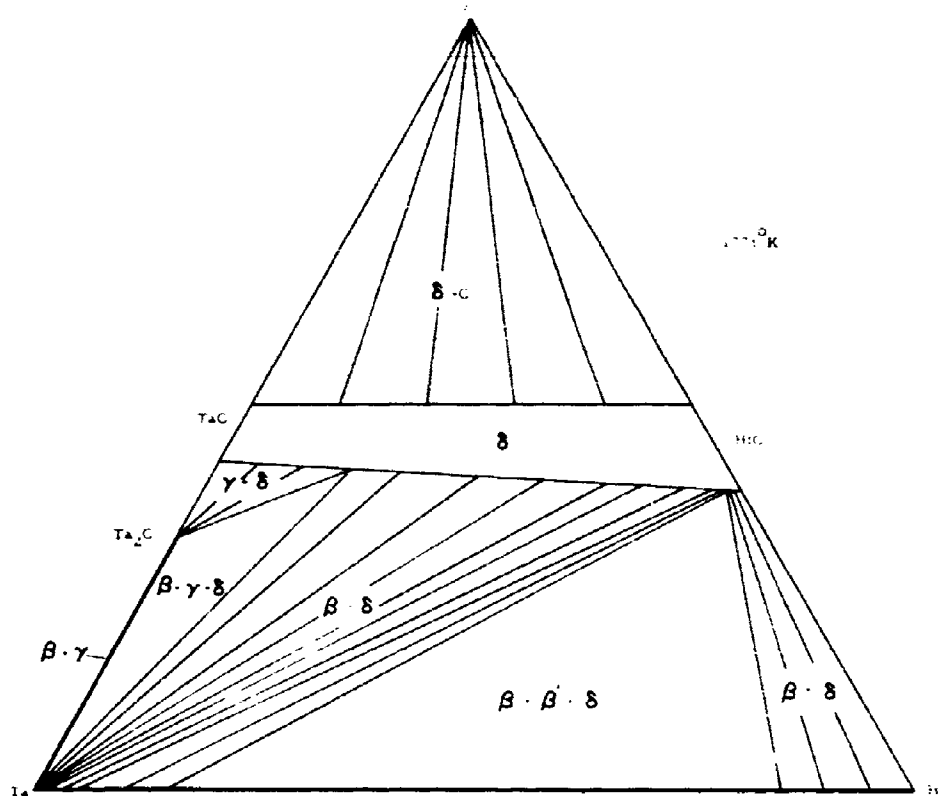


Figure 22. Calculated Phase Equilibria in the System Ta-Hf-C Using the Simplified Method at 1773°K.

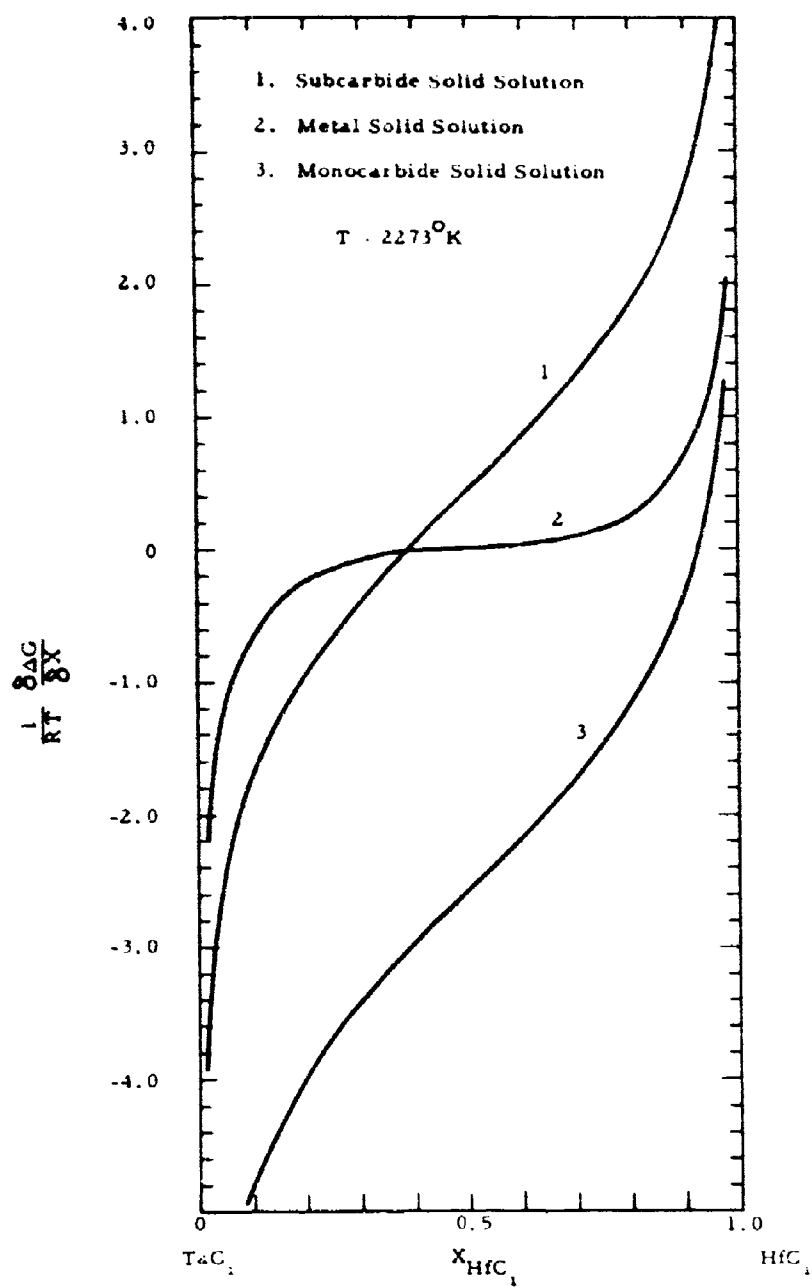


Figure 23. Concentration Free-Energy-Gradient Curves for the Metal, Subcarbide and Monocarbide Solid Solutions.

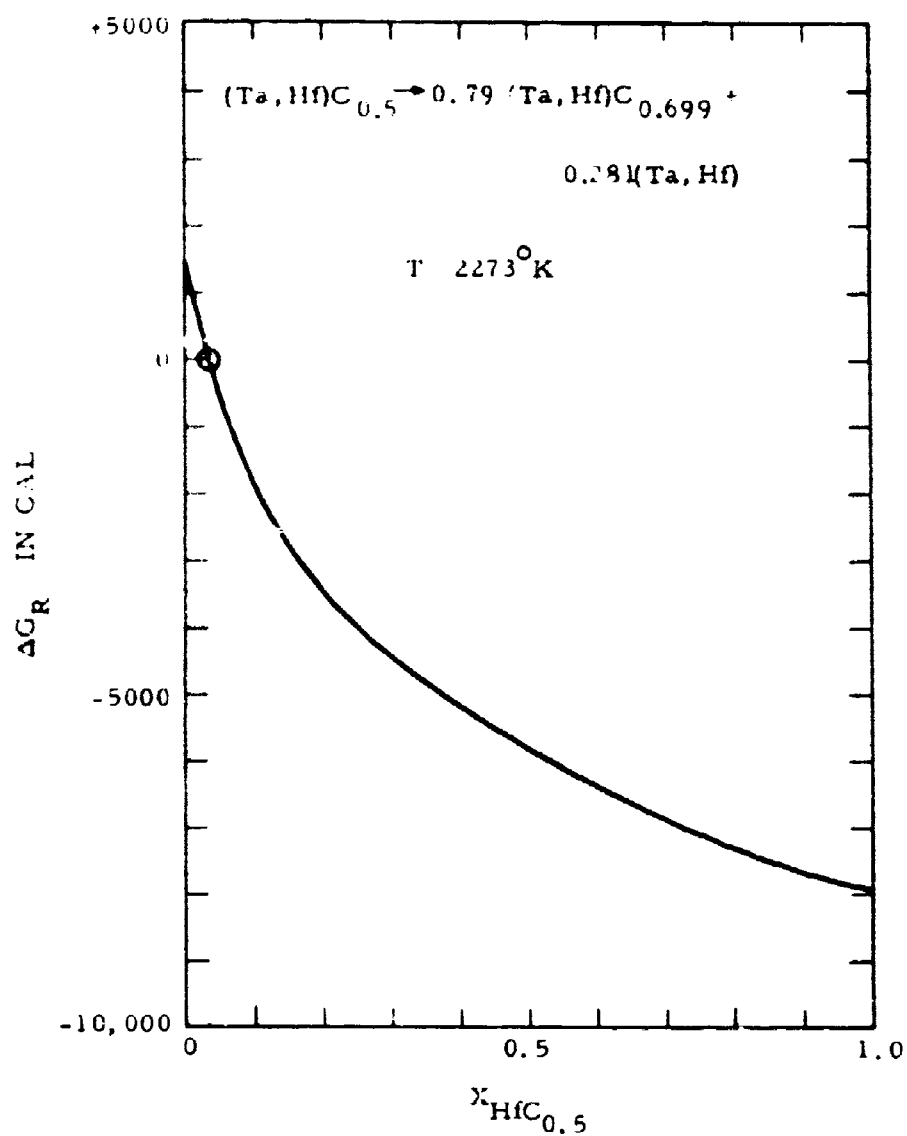


Figure 24. Integral Free Energy of Decomposition of the Subcarbide Phase into the Metal and Monocarbide Phases at 2273°K .

IV. DISCUSSION

The method described in this report has demonstrated that the phase equilibria in three-component systems can be adequately predicted from binary data based on the first principle provided that the Gibbs free energies of formation of all the binary phases are accurately known as a function of composition and temperature. Moreover, one must also know the solution behaviors of the ternary alloys. It has been demonstrated previously^(2, 3), that for the interstitial type of solid solution such as the transition metal carbides, the regular solution theory with proper values of the interaction parameters, is adequate in most cases.

The general method also demonstrates that the simplified method originally developed by Rudy for predicting phase equilibria in three-component systems is sufficiently accurate. In cases where the homogeneous ranges of the ternary solid solutions with respect to the interstitial component such as carbon are small, the simplified method would predict the identical results as the general method. Only, when the homogeneous ranges of a ternary solid solution with respect to the interstitial element change drastically with the metal exchange, will there be a difference between the phase diagrams calculated using the two different methods. In practice, the phase equilibria in a ternary system predicted by the simplified method are sufficiently accurate in most cases.

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APPENDIX I

COMPUTER PROGRAMS FOR TERNARY PHASE
DIAGRAM CALCULATIONS (Ray Marler)

```

$IBFTC K=1      FULIST
      DIMENSION X(50),Y(50),A3(3),A4(3),TITLE(13)
      NAMLIST/INPUT/NOXYS,IPRINT,CASE,DUMP,XLIM,R,T,EPSP,EPSPP,A3,A4,
      1X,Y,K1,K2
      NAMLIST/DTADMP/LINE,K,J,XP,YP,XPP,YPP,ZPP,DG,DG3,DG4,GNU1,GNU2,
      1FXP,FYP,DG1,C1,C2,FC1,FC2,DG2
1  FORMAT(1H139X53H A E R O J E T - G E N E R A L   C O R P O R A T I
10 N/1H039X53H C O M P U T I N G   S C I E N C E S   D I V I S I O N
2/1H050X31H S A C R A M E N T O   P L A N T//1H057X17H P R O G R A M
3  K/1H027X77H T W O - P H A S E   E Q U I L I B R I U M   I N   T E
4 R N A R Y   S Y S T E M/16H0C U S T O M E R 97X19H P R O G R A M M
5 E R/12H0Y. A. CHANG109X11H R. H. MARLER//)
      READ(5,17)TITLE
2  READ (5,INPUT)
      WRITE(6,1)
      WRITE(6,18)TITLF
      WRITE(6,INPUT )
      LIM = XLIM + .005
      NDUMP1= DUMP
      NDUMP2 = INT(DUMP*XLIM+.005) - NDUMP1*LIM
      RT = R*T
      WRITE(6,1)
      WRITE(6,18)TITLF
      DO 14 I = 1, NOXYS
      WRITE(6,16)X(I),Y(I)
      PASS = 1.
      L = 1
      LINF = 1
      LIMX = XLIM * X(I) + .005
      BLIMX = LIMX
      JMAX = LIM - LIMX
      DO 12 K = K1,K2
      CAY = K
      XPP = CAY/XLIM
      DO 12 J = 1, JMAX
      XJ = J
      XP = (BLIMX + XJ)/XLIM
      ZPP = (XP - XPP)*(1.-X(I)-Y(I))/(XP - X(I))
      IF(ZPP.GE.1..OR.ZPP.LE.0..OR.XP.FQ.XPP.OR.XP.EQ.X(I))GO TO 12
      DG3 = ((A3(3)*ZPP+A3(2))*ZPP+A3(1))/(1.-ZPP)
      DG4 = ((A4(3)*ZPP+A4(2))*ZPP+A4(1))/(1.-ZPP)
      GNU1 = (X(I)-XPP)/(XP-XPP)
      GNU2 = (XP-X(I))/(XP-XPP)
      IF(GNU1.LT.0..OR.GNU1.GT.1..OR.GNU2.LT.0..OR.GNU2.GT.1.)GO TO 12
      YP = 1.-XP
      YPP = 1. -XPP - ZPP
      CALL XLNX(XP,FXP,$12)
      CALL XLNX(YP,FYP,$12)
      DG1 = (FXP+FYP)*RT+XP*YP*EPSP
      C1 = XPP/(1.-ZPP)
      C2 = YPP/(1.-ZPP)
      CALL XLNX(C1,FC1,$12)
      CALL XLNX(C2,FC2,$12)
      DG2=((FC1+FC2)*RT+C1*C2*EPSPP+C1*DG3+C2*DG4)*(1.-ZPP)
      DG =GNU1*DG1+GNU2*DG2
      IF(DG.GE.0.)GO TO 12
      IF(PASS.NE.1.)GO TO 5
      PASS = 0.
      GO TO 6

```

```

5 IF (DG = DGOLD)6,8,8
6 DGOLD = DG
  XPS = XP
  YPS = YP
  XPPS= XPP
  YPPS= YPP
  ZPPS= ZPP
  LSAVE = LINE
8 IF(NDUMP1.NE.K.OR.NDUMP2.NE.J)GO TO 9
  WRITE (6,DTADMP)
  GO TO 11
9 IF(IPRINT.EQ.0)WRITE(6,10)LINE,XP,YP,XPP,YPP,ZPP,DG
10 FORMAT(1H 15X14,6E16.8)
11 LINE = LINE + 1
12 CONTINUE
  WRITE(6,10)LSAVE,XPS,YPS,XPPS,YPPS,ZPPS,DGOLD
14 CONTINUE
  CASE = CASE - 1.
  IF(CASE.GT.0.)GO TO 2
15 STOP
16 FORMAT(1H019X 4HX = E15.8,10X,4HY = E15.8/1H 15X4HLINE7X2HXP14X
  12HYP13X3HXPP13X3HYPP13X3HZPP12X5HDEL G)
17 FORMAT(13A6)
18 FORMAT(1H027X13A6)
  END

```

```

$IRFEC K-1-A FULIST
  DIMENSION X(50),Y(50),TITLE(13),VA(5),VB(5),RA(5),RB(5)
  NAMELIST/INPUT/NOXYS,IPRINT,CASE,DUMP,XLIM,R,T,EPSP,EPSP,VA,VB,
1    X,Y,K1,K2,D3,D4,RA,RB,DEACV,DEBCV,DCACU,DGBCU
  NAMELIST/DTADMP/K,J,XP,YP,XPP,YPP,ZPP,DG,DGACV,DGBCV,GNU1,GNU2,
1FXP,FYP,DG1,C1,C2,FC1,FC2,DG2
1 FORMAT(1H139X53H A E R O J E T - G E N E R A L C O R P O R A T I
10 N/1H039X53H C O M P U T I N G S C I E N C E S D I V I S I O N
2/1H050X31H S A C R A M E N T O P L A N T//1H057X17H P R O G R A M
3   K/1H027X77H T W O - P H A S E E Q U I L I B R I U M I N T E
4   R N A R Y S Y S T E M/16H0C U S T O M E R 97X19H P R O G R A M M
5   E R/12H0Y. A. CHANG109X11HR.H. MARLER//)
  READ(5,17)TITLE
2 READ(5,INPUT)
  WRITE(6,1)
  WRITE(6,18)TITLE
  WRITE(6,INPUT)
  LIM = XLIM + .005
  NDUMP1 = DUMP
  NDUMP2 = INT(DUMP*XLIM+.005) - NDUMP1*LIM
  FLAG = NDUMP1
  RT = R*T
  WRITE(6,1)
  WRITE(6,18)TITLE
  DO 14 I = 1, NOXYS
    WRITE(6,16)X(I),Y(I)
    PASS = 1.
    LIMX = XLIM * X(I) + .005
    BLIMX = LIMX
    JMAX = LIM - LIMX
    DO 12 K = K1,K2
      CAY = K
      XPP = CAY/XLIM
      DO 12 J = 1, JMAX
        XJ = J
        XP = (BLIMX + XJ)/XLIM
        IF(XP.EQ.XPP.OR.XP.EQ.X(I))GO TO 12
        ZPP = (XP - XPP)*(1.-X(I)-Y(I))/(XP - X(I))
        IF(ZPP.EQ..5)ZPP = .499
        IF(ZPP.GT.D4.OR.ZPP.LT.D3)GO TO 12
        CALL DLGC(DGACV,R,T,ZPP,VA,RA,DEACV,FLAG,$12)
        CALL DLGC(DGBCV,R,T,ZPP,VB,RB,DEBCV,FLAG,$12)
        GNU1 = (X(I)-XPP)/(XP-XPP)
        GNU2 = (XP-X(I))/(XP-XPP)
        IF(GNU1.LT.0..OR.GNU1.GT.1..OR.GNU2.LT.0..OR.GNU2.GT.1.)GO TO 12
        YP = 1.-XP
        YPP = 1.-XPP - ZPP
        CALL XLNX(XP,FXP,$12)
        CALL XLNX(YP,FYP,$12)
        DG1 = (FXP+FYP)*RT+XP*YP*EPSP+DGACU*XP+DGBCU*YP
        C1 = XPP/(1.-ZPP)
        C2 = YPP/(1.-ZPP)
        CALL XLNX(C1,FC1,$12)
        CALL XLNX(C2,FC2,$12)
        DG2 = ((FC1+FC2)*RT + C1*C1*EPSP + C2*DGBCV + C1*DGACV)*(1.-ZPP)
        DG = GNU1*DG1+GNU2*DG2
        IF(DG.GT.0.)GO TO 12
        IF(PASS.NE.1.)GO TO 4
        PASS = 0.

```

```

      GO TO 6
5  IF (DG - DGOLD)16,R,8
6  DGOLD = DG
   XPS = XP
   YPS = YP
   XPPS = XPP
   YPPS = YPP
   ZPPS = ZPP
8  IF(NDUMP1.NE.K.OR.NDUMP2.NE.J)GO TO 9
   WRITE (6,DTADMP)
   FLAG = 0
   GO TO 12
9  IF(IPRINT.EQ.0)WRITE(6,10)      XP,YP,XPP,YPP,ZPP,DG
10 FORMAT(1H 19X5F16.8,F16.4)
12 CONTINUE
   WRITE(6,10)      XPS,YPS,XPPS,YPPS,ZPPS,DGOLD
14 CONTINUE
   CASE = CASE - 1.
   IF(CASE.GT.0.)GO TO 2
15 STOP
16 FORMAT(1H023X4HX = F10.8,5X,4HY = F10.8/1H 26X2HXPI4X
        12HYP13X3HXPP13X3HYPP13X3HZPP12X5HDEL G)
17 FORMAT(13A6)
18 FORMAT(1H027X13A6)
   END

```

```

$IRFC X=2      FULIST
      DIMENSION X(50),Y(50),Z(50),TITLE(13),CDG3(3),CDG4(3),CDG5(3),
      1CDG6(3)
      NAMELIST/INPUT/      A,B,C,D,R,T,DELTA,EPSP,EPSP,CDG3,CDG4,
      1CDG5,CDG6,X,Y,Z
1  FORMAT(1H139X53HA E R O J E T - G E N E R A L   C O R P O R A T I
10 N/1H039X53HC O M P U T I N G   S C I E N C E S   D I V I S I O N
2/1H050X31HS A C R A M E N T O   P L A N T//1H057X17HP R O G R A M
3  K/1H019X93HG E N E R A L   T W O - P H A S E   E Q U I L I B R I
4 U M   I N   T E R N A R Y   S Y S T E M/16H0C U S T O M E R 97X
519HP R O G R A M M E R/12H0Y   A. CHANG109X11HR:H. MARLER//)
      READ(5,*)TITLE,ID
2  FORMAT(13A6,I2)
2  READ (5,INPUT)
      WRITE (6,1)
      WRITE(6,4)TITLE,ID
4  FORMAT(1H026X13A6,25X12)
      WRITE (6,INPUT)
      WRITE(6,1)
      WRITE(6,16)TITLE
16 FORMAT(1H026X13A6// 7X1HX12X1HY12X1HZ11X2HXP11X2HYP11X2HZP11X3HXP
111X3HYPP11X3HZPP 9X7HDELTA G/)
      RT = R*T
      DO 14 I = 1,50
      IF(X(I).EQ.0..AND.Y(I).EQ.0..AND.Z(I).EQ.0.)GO TO 15
      IPASS = 1
17 IF(A.EQ.X(I))A = X(I)+DELTA/10.
      XPP = A
5  IF(XPP - X(I)) 6,13,7
6  XP = X(I) + DELTA
      XPMAX = 1.
      GO TO 8
7  XP = 0.
      XPMAX = X(I)
8  ZP = 0
12 YP = 1.-XP-ZP
      IF(XP.EQ.XPP)GO TO 11
      GNU1 = (X(I)-XPP)/(XP-XPP)
      IF(GNU1.GE.1..OR.GNU1.LT.0.)GO TO 11
      GNU2 = 1.-GNU1
      YPP = (Y(I)-GNU1*YP)/GNU2
      ZPP = 1.-XPP-YPP
      IF(ZPP.GE.1..OR.ZPP.LT.0.)GO TO 11
      CALL CUBIC(CDG3,ZPP,DG3,$11)
      CALL CUBIC(CDG4,ZPP,DG4,$11)
      U1 = XPP/(1.-ZPP)
      U2 = YPP/(1.-ZPP)
      CALL XLNX(U1,FU1,$11)
      CALL XLNX(U2,FU2,$11)
      DG2=((FU1+FU2)*RT+U1*U2*EPSP +U2*DG4 + U1*DG3)*(1.-ZPP)
      CALL CUBIC(CDG5,ZP,DG5,$11)
      CALL CUBIC(CDG6,ZP,DG6,$11)
      U1= XP/(1.-ZP)
      U2= YP/(1.-ZP)
      CALL XLNX(U1,FU1,$11)
      CALL XLNX(U2,FU2,$11)
      DG1=((FU1+FU2)*RT + U1*U2*EPSP +U2*DG6 + U1*DG5)*(1.-ZP)
      DG = GNU1*DG1 + GNU2 * DG2
      IF(IPASS.EQ.0)GO TO 19

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```

      IPASS = 0
      DGS = DG
19  IF(DG.GE.DGS)GO TO 9
      DGS = DG
      XPS = XP
      YPS = YP
      XPPS = XPP
      YPPS = YPP
      ZPS = ZP
      ZPPS = ZPP
9   IF(ID.NE.0)WRITE(6,10)X(I),Y(I),Z(I),XP,YP,ZP,XPP,YPP,ZPP,DG
10  FORMAT(1H 9F13.8,F13.4)
11  ZP = ZP + DELTA
      IF(ZP.LE.0)GO TO 12
      XP = XP + DELTA
      IF(XP.LT.XPMAX)GO TO 8
13  XPP = XPP + DELTA
      IF(XPP.LE.0)GO TO 5
      WRITE(6,10)X(I),Y(I),Z(I),XPS,YPS,ZPS,XPPS,YPPS,ZPPS,DGS
14  CONTINUE
15  GO TO 2
      END

```



```

SIRFTC K-2-A FULIST
  DIMENSION X(50),Y(50),Z(50),TITLE(13),VACV(5),VBCV(5),VACU(5),
1    VBCU(5),RACV(5),RACU(5),RBCV(5),RBCU(5)
  NAMELIST/INPUT/ A,B,C,D,E,F,R,T,DELTA,EPSP,EPSP,DEACV,DEBCV,
1    IDEACU,DEBCU,VACV,VBCV,VACU,VBCU,ACV,RACV,RACU,RBCU,X,Y,Z
2    FORMAT(1H139X53H A E R O J E T - G E N E R A L C O R P O R A T I
10   N/1H039X53H C O M P U T I N G S C I E N C E S D I V I S I O N
2/1H050X31H S A C R A M E N T O P L A N T//1H057X17H P R O G R A M
3    /1H019X93H G E N E R A L T W O - P H A S E E Q U I L I B R I
4    U M I N T E R N A R Y S Y S T E M/16H0C U S T O M E R 97X
519H P R O G R A M M E R/12H0Y. A. CHAN5109X11HR.H. MARLER//)
  READ(5,3)TITLE,ID
3    FORMAT(13A6,I2)
2    READ(5,INPUT)
  WRITE(6,1)
  WRITE(6,4)TITLE,ID
4    FORMAT(1H026X13A6,25X12)
  WRITE(6,INPUT)
  WRITE(6,1)
  WRITE(6,16)TITLE
16   FORMAT(1H026X13A6// 7X1HX12X1HY12X1HZ11X2HXP11X2HYP11X2HZP11X3HXP
111X3HYPP11X3HZPP 9X7HDELTA G/)
  FLAG = ID/10
  RT = R*T
  DO 14 I = 1,50
  IF(X(I).EQ.0..AND.Y(I).EQ.0..AND.Z(I).EQ.0.)GO TO 15
  IPASS = 1
  XPP = A
  DO 17 IXPP=1,1000
  IF(XPP-X(I))6,13,7
6    XP = X(I) + DELTA
  XPMAX = F
  GO TO 8
7    XP = E
  XPMAX = X(I)
8    DO 18 IXP=1,1000
  ZP=C
  DO 22 IZP=1,1000
  YP=1.-XP-ZP
  IF(XP.EQ.XPP)GO TO 11
  GNU1 = (X(I)-XPP)/(XP-XPP)
  IF(GNU1.GE.1..OR.GNU1.LT.0.)GO TO 11
  GNU2 = 1.-GNU1
  YPP = (Y(I)-GNU1*YP)/GNU2
  ZPP = 1.-XPP-YPP
  IF(ZPP.GE.1..OR.ZPP.LT.0.)GO TO 11
  CALL DLGC(DGACV,R,T,ZPP,VACV,RACV,DEACV,FLAG,$11)
  CALL DLGC(DGBCV,R,T,ZPP,VACV,RBCV,DEBCV,FLAG,$11)
  U1 = XPP/(1.-ZPP)
  U2 = YPP/(1.-ZPP)
  CALL XLNX(U1,FU1,$11)
  CALL XLNX(U2,FU2,$11)
  DG2=((FU1+FU2)*RT+U1*U2*EPSP+U2*DGBCV+U1*DGACV)*(1.-ZPP)
  CALL DLGC(DGACU,R,T,ZP,VACU,RACU,DEACU,FLAG,$11)
  CALL DLGC(DGBCU,R,T,ZP,VBCU,RBCU,DEBCU,FLAG,$11)
  U1= XP/(1.-ZP)
  U2= YP/(1.-ZP)
  CALL XLNX(U1,FU1,$11)
  CALL XLNX(U2,FU2,$11)

```

```

      DG1 = ((FU1+FU2)*RT+U1*U2*EPSP+U2*DGRCU+U1*DGACU)*(1.-ZP)
      DG = GNU1*DG1 + GNU2 * DG2
      IF(IPASS.EQ.0)GO TO 19
      IPASS = 0
      DGS = DG
19  IF(DG.GE.DGS)GO TO 4
      DGS = DG
      XFS = XF
      YFS = YF
      XPPS = XPP
      YPPS = YPP
      ZPS = ZP
      ZPPS = ZPP
      9  IF(ID.NE.0)WRITE(6,10)X(1),Y(1),Z(1),XF,YF,ZP,XPP,YPP,ZPP,DG
10  FORMAT(1H 9F15.5,F15.4)
11  ZP = ZP + DELTA
      IF(ZP.GT.1)GO TO 12
22  CONTINUE
      WRITE(6,23)
23  FORMAT(25HOTHER ZP LOOP WAS EXCEEDED)
      GO TO 5
12  XP = XP+DELTA
      IF(XP.GE.XPMAX)GO TO 13
18  CONTINUE
      WRITE(6,20)
20  FORMAT(25HOTHER XP LOOP WAS EXCEEDED)
      GO TO 5
13  XPP = XPP + DELTA
      IF(XPP.GT.3)GO TO 5
17  CONTINUE
      WRITE(6,21)
21  FORMAT(26HOTHER XPP LOOP WAS EXCEEDED)
      5  WRITE(6,10)X(1),Y(1),Z(1),XF,YF,ZP,XPP,YPP,ZPP,DGS
14  CONTINUE
15  GO TO 2
      END

```

51910 4-3 FOLIST

```

DIMENSION TITLE(13)
COMMON CDGACV(3),CDGBCV(3),CDGACW(3),CDGBCW(3)
NAMELIST/INPUT/R1,B2,DELTA,X,Y,Z,XP,YP,ZP,XPP,YPP,ZPP,R,T,M,
1CDGACV,CDGBCV,CDGACW,CDGBCW,EPSP,EPSP,EPSP
1 FORMAT(1H139X53H)A L R O J E T - G E N E R A L C O R P O R A T I
10 N/1H039X53H C O M P U T I N G S C I E N C E S D I V I S I O N
2/1H050X31H S A C R A M E N T O P L A N T/1H057X17H P R O G R A M
3 K/1H019X23H G E N E R A L T W O - P H A S E E Q U I L I B R I
4 U M I N T E R N A R Y S Y S T E M/16H0 C U S T O M E R 97X
519HP R O G R A M M E R/12H O Y . A . C H A N G 109X11H R . H . M A R L E R / / )
READ(5,3)TITLE,ID
3 FORMAT(13A6,I2)
2 READ (5,INPUT)
WRITE (6,1)
WRITE(6,4)TITLE,ID
4 FORMAT(1H026X13A6,25X12)
WRITE (6,INPUT)
WRITE(6,1)
WRITE(6,5)TITLE
RT=R*T
CALL DGACVS(DGACV,ZPP,$11)
CALL DGBCVS(DGBCV,ZPP,$11)
U1=XP/(1.-ZP)
U2=YP/(1.-ZP)
CALL XLNX(U1,FU1,$11)
CALL XLNX(U2,FU2,$11)
DG1 = (FU1+FU2)*RT + EPSP*U1*U2
U1=XPP/(1.-ZPP)
U2=YPP/(1.-ZPP)
CALL XLNX(U1,FU1,$11)
CALL XLNX(U2,FU2,$11)
DG2 = ((FU1+FU2)*RT + EPSP*U1*U2 + DGBCV*U2 + DGACV*U1)*(1.-ZPP)
13 IPASS=1
DYP = YP-Y
DYPP=YPP-Y
DZP = ZP-Z
DZPP=ZPP-Z
AREA2 =DYPP*DZP - DYP*DZPP
ZPPP= R1
7 YPPP=0.
YPPDMX=1.-ZPPP
DZPPP=ZPPP-Z
8 DYPPP=YPPP-Y
AREA1 =DYP*DZPPP-DYPPP*DZP
AREA3 =DYPPP*DZPP - DYPP*DZPPP
IF(.NOT.(AREA1.LT.0..AND.AREA2.LT.0..AND.AREA3.LT.0..OR.AREA1.GT.
10..AND.AREA2.GT.0..AND.AREA3.GT.0.))GO TO 11
XPPP=1.-YPPP-ZPPP
CALL DGACWS(DGACW,ZPPP,$11)
CALL DGBCWS(DGBCW,ZPPP,$11)
U1=XPPP/(1.-ZPPP)
U2=YPPP/(1.-ZPPP)
CALL XLNX(U1,FU1,$11)
CALL XLNX(U2,FU2,$11)
DG3 = ((FU1+FU2)*RT+EPSP*U1*U2 + DGBCW*U2 + DGACW*U1)*(1.-ZPPP)
D = (YPP - YP)*(ZPPP- ZP) - (ZPP - ZP) * (YPPP- YP)
IF(D.EQ.0.)GO TO 11
G'U1 = ((YPP-Y)*(ZPPP-Z) - (ZPP-Z)*(YPPP-Y))/D

```

```

IF(GNU1.LE.0..OR.GNU1.GT.1.)GO TO 11
GNU2 = ((Y-YP)*(ZPPP-ZP) - (Z-ZP)*(YPPP-YP))/D
IF(GNU2.LE.0..OR.GNU2.GT.1.)GO TO 11
GNU3 = 1.-GNU1-GNU2
DG = GNU1* DG1 + GNU2 *DG2 + GNU3*DG3
IF(IPASS.EQ.0)GO TO 9
IPASS = 0
DGS = DG
9 IF(DG.GE.DGS)GO TO 10
DGS = DG
XPPPS = XPPP
YPPPS = YPPP
ZPPPS = ZPPP
10 IF(ID.NE.0)WRITE(6,14)X,Y,Z,XP,YP,ZP,XPP,YPP,ZPP,XPPP,YPPP,ZPPP,DG
11 YPPP = YPPP + DELTA
IF(YPPP.LE.YPPPMX)GO TO 8
ZPPP = ZPPP + DELTA
IF(ZPPP.LE.B2) GO TO 7
WRITE(6,14)X,Y,Z,XP ,YP ,ZP ,XPP ,YPP ,ZPP ,
1XPPPS,YPPPS,ZPPPS,DGS
M = M -1
IF(M.LT.0)GO TO 2
IF(DGS.GE.0.)GO TO 12
B1 =AMAX1(B1,DGS-DELTA)
B2 =AMIN1(B2,DGS+DELTA)
12 DELTA = DELTA/10.
GO TO 13
14 FORMAT(1H 12F10.7,F10.3)
5 FORMAT(1H026X
1 13A6//130H X Y Z XPPP XP YPPP Y
1P ZP XPP YPP ZPP XPPP YPPP
2 ZPPP DELTA G/)
END

```

SIBFTC K-3-A FULIST

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    DIMENSION TITLE(13),PACV(5),RBCV(5),RACW(5),RBCW(5),VACV(5),
    1 VBCV(5),VACW(5),VBCW(5)
    NAMELIST/INPUT/B1,B2,DELTA,X,Y,Z,XP,YP,ZP,XPP,YPP,ZPP,R,T,M,EPSP,
    1 EPSPP,EPSPPP,DEACV,DERCV,DEACW,DEBCW,VACV,VBCV,VACW,VBCW,
    2 RACV,RBCV,RACW,RBCW,DGACU,DGRCU
    1 FORMAT(1H139X53H A E R O J E T - G E N E R A L C O R P O R A T I
    10 N/1H039X53H C O M P U T I N G S C I E N C E S D I V I S I O N
    2/1H050X31H S A C R A M E N T O P L A N T//1H057X17H P R O G R A M
    3 K/1H019X93H G E N E R A L T W O - P H A S E E Q U I L I B R I
    4 U M I N T E R N A R Y S Y S T E M/16H0C U S T O M E R 97X
    519H P R O G R A M M E R/12HOY. A. CHANG109X11HR.H. MARLER//)
    READ(5,3)TITLE,ID
    3 FORMAT(13A6,I2)
    2 READ(5,INPUT)
    WRITE(6,1)
    WRITE(6,4)TITLE,ID
    4 FORMAT(1H026X13A6,25X12)
    WRITE(6,INPUT)
    WRITE(6,1)
    WRITE(6,5)TITLE
    FLAG = ID/10
    RT=R*T
    CALL DLGC(DGACV,R,T,ZPP,VACV,RACV,DEACV,FLAG,$11)
    CALL DLGC(DGBCV,R,T,ZPP,VBCV,RBCV,DEACV,FLAG,$11)
    U1=XP/(1.-ZP)
    U2=YP/(1.-ZP)
    CALL XLNX(U1,FU1,$11)
    CALL XLNX(U2,FU2,$11)
    DG1 = (FU1+FU2)*RT + EPSP*U1*U2+DGACU*XP+DGRCU*YP
    U1=XPP/(1.-ZPP)
    U2=YPP/(1.-ZPP)
    CALL XLNX(U1,FU1,$11)
    CALL XLNX(U2,FU2,$11)
    DG2 = ((FU1+FU2)*RT + EPSP*U1*U2 + DGBCV*U2 + DGACV*U1)*(1.-ZPP)
    13 IPASS=1
    DYP = YP-Y
    DYPP=YPP-Y
    DZP = ZP-Z
    DZPP=ZPP-Z
    AREA2 =DYP*DZP - DYP*DZPP
    ZPPP= 0
    7 YPPP = 0.
    YPPMX=1.-ZPPP
    DZPPP=ZPPP-Z
    9 DYPPP=YPPP-Y
    AREA1 =DYP*DZPPP-DYPPP*DZP
    AREA3 =DYPPP*DZPP - DYPP*DZPPP
    IF(.NOT.(AREA1.LT.0..AND.AREA2.LT.0..AND.AREA3.LT.0..OR.AREA1.GT.
    10..AND.AREA2.GT.0..AND.AREA3.GT.0.))GO TO 11
    XPPP=1.-YPPP-ZPPP
    CALL DLGC(DGACW,R,T,ZPPP,VACW,RACW,DEACW,FLAG,$11)
    CALL DLGC(DGRCW,R,T,ZPPP,VBCW,RBCW,DERCW,FLAG,$11)
    U1=XPPP/(1.-ZPPP)
    U2=YPPP/(1.-ZPPP)
    CALL XLNX(U1,FU1,$11)
    CALL XLNX(U2,FU2,$11)
    DG3 = ((FU1+FU2)*RT+EPSP*U1*U2 + DGRCW*U2 + DGACW*U1)*(1.-ZPPP)
    D = (YPP - YP)*(ZPPP - ZP) - (ZPP - ZP) * (YPPP - YP)

```

```

IF(D.EQ.0.)GO TO 11
GNU1 = ((YPP-Y)*(ZPPP-Z) - (ZPP-Z)*(YPPP-Y))/D
IF(GNU1.LE.0..OR.GNU1.GT.1.)GO TO 11
GNU2 = ((Y-YP)*(ZPPP-ZP) - (Z-ZP)*(YPPP-YP))/D
IF(GNU2.LE.0..OR.GNU2.GT.1.)GO TO 11
GNU3 = 1.-GNU1-GNU2
DG = GNU1* DG1 + GNU2 *DG2 + GNU3*DG3
IF(IPASS.EQ.0)GO TO 9
IPASS = 0
DGS = DG
9 IF(DG.GT.DGS)GO TO 10
DGS = DG
XPPPS = XPPP
YPPPS = YPPP
ZPPPS = ZPPP
10 IF(ID.NE.0)WRITE(6,14)X,Y,Z,XP,YP,ZP,XPP,YPP,ZPP,XPPS,YPPS,ZPPS,DG
11 YPPP = YPPP + DELTA
IF(YPPP.LE.YPPPMX)GO TO 8
ZPPP = ZPPP + DELTA
IF(ZPPP.LE.B2) GO TO 7
WRITE(6,14)X,Y,Z,XP,YP,ZP,XPP,YPP,ZPP,XPPS,YPPS,ZPPS,DGS
1XPPPS,YPPPS,ZPPPS,DGS
M = M -1
IF(M.LT.0)GO TO 2
IF(DGS.GE.0.)GO TO 12
B1 =AMAX1(B1,DGS-DELTA)
B2 =AMIN1(B2,DGS+DELTA)
12 DELTA = DELTA/10.
GO TO 13
14 FORMAT(1H 12F10.7,F10.3)
5 FORMAT(1H025X
1      13A6//130H      X      Y      Z      XPP      XP      Y
1P      ZP      XPP      YPP      ZPP      XPPS      YPPS
2      ZPPS      DELTA G/)
END

```

\$IBLDR XLNXF	12/17/65	XLNX0000
\$TEXT XLNXF	12/17/65	XLNX0001
*N ((X\$7V*7'7-5 00 80 9 9 94 8 93 77 7749G405 Z4 8 93 'G '5 'XLNX0002		
*N9(('*XV*7(*7-5 5 ' 74+03' W= ' 7 9 5 Z *)P0 ')4'G47'4'04'74'XLNX0003		
N8V'7V*X(*7-74 04'74774 ' '5 7 'G 074074'74'449' ' '7' ' '7447' 'XLNX0004		
59(2'/ ' '5 ' ' 'XLNX0005		
\$CDICT XLNXF	12/17/65	XLNX0006
/ ((0' 1')P 0 0 9*)P '*)P-6 P*}-		XLNX0007
\$DKEND XLNXF	12/17/65	XLNX0008
\$IBFTC CUBICF NOLIST		
SUBROUTINE CUBIC(COEF,X,Y,*)		
DIMENSION COEF(3)		
IF(X.EQ.1.)RETURN 1		
Y = ((X*COEF(3)+COEF(2))*X+COEF(1))/(1.-X)		
RETURN		
END		

```

SIBFTC DGACVF FULIST
  SUBROUTINE DGACVS(DGACV,ZPP,*)
  COMMON   CDGACV(3),CDGBCV(3),CDGACW(3),CDGBCW(3)
  CALL CUBIC(CDGACV,ZPP,DGACV,$10)
  RETURN
10 RETURN 1
  END

SIBFTC DGBCVF FULIST
  SUBROUTINE DGBCVS(DGBCV,ZPP,*)
  COMMON   CDGACV(3),CDGBCV(3),CDGACW(3),CDGBCW(3)
  CALL CUBIC(CDGBCV,ZPP,DGBCV,$10)
  RETURN
10 RETURN 1
  END

SIBFTC DGACWF FULIST
  SUBROUTINE DGACWS(DGACW,ZPPP,*)
  COMMON   CDGACV(3),CDGBCV(3),CDGACW(3),CDGBCW(3)
  CALL CUBIC(CDGACW,ZPPP,DGACW,$10)
  RETURN
10 RETURN 1
  END

SIBFTC DGBCWF FULIST
  SUBROUTINE DGBCWS(DGBCW,ZPPP,*)
  COMMON   CDGACV(3),CDGBCV(3),CDGACW(3),CDGBCW(3)
  CALL CUBIC(CDGBCW,ZPPP,DGBCW,$10)
  RETURN
10 RETURN 1
  END

```



```

$IBFTC DELGC FULIST
  SUBROUTINE DLGC (DGC,R,T,ARG,V,ARE,DELE,FLAG,*)
  DIMENSION V(5),ARE(5)
  GC = ARE(5)*T + ARE(4)
  DGFC = (ALOG10(T)*ARE(2)+ARE(3))*T + ARE(1)
  CALL DGXS(ARG,DELE,R,T,DELGXS,FLAG,$2)
  DGC=(((ARG*V(5)+V(4))*ARG+V(3))*ARG+V(2))*ARG+V(1)+(1.-2.*ARG)*
1 GC+(1.-ARG)*DGFC+DELGXS)/(1.-ARG)
  IF(FLAG.GT.0.)WRITE(6,1)GC,DGFC,DGC
1 FORMAT( 6H GC = E15.8,5X 7HDGFC = E15.8,5X6HDGC = E15.8)
  RETURN
2 RETURN1
  END
$IBFTC DLGXS FULIST
  SUBROUTINE DGXS(X,DELE,R,T,DELGXS,FLAG,*)
  RT=R*T
  IF(DELE)10,5,1
1 W=DELE/RT
  EXPW = EXP(W)
  EXPNW =1./EXPW
  CALL XSUBAB(X,EXPNW,XA,XB,FLAG,$10)
  CALL PRELIM(XA,XB,EXPNW,EXPW,SMALLR,S,FLAG)
  CALL DELGCX(DELE,RT,XA,XB,SMALLR,S,DLGCXS,FLAG)
  CALL DELGMX(X,XA,XB,RT,DELE,DLGCXS,DGMEXS,FLAG)
  CONJXA=1.-XA
  CONJXB=1.-XB
  CALL XLNX(XA,FXA,$10)
  CALL XLNX(CONJXA,FCNJXA,$10)
  CALL XLNX(XB,FXB,$10)
  CALL XLNX(CONJXB,FCNJXB,$10)
  DELGXS=((FXA+FXB+FCNJXA-FCNJXB)*RT +XB*DELE)*(1.-X)/2.
  GO TO 9
5 CONJX=1.-X
  CALL XLNX (X,FX,$10)
  CALL XLNX (CONJX,FCONJX,$10)
  UX=1.-2.*X
  CALL XLNX(UX,FUX,$10)
  DELGXS =(FUX-FCONJX+ FX)*RT
9 IF(FLAG.GT.0.)WRITE(6,11)DELGXS
  RETURN
10 RETURN 1
11 FORMAT(10H DELGXS = E15.8)
  END

```

```

SEXECUTE      IRJOB
SIRJOB A48052  MAP
SIBFTC TAB    FULIST
      DIMENSION DELTAE(10), TEE(10)
1 READ(5,100) IDE, IT, (DELTAE(I), I=1, IDE), (TEE(I), I=1, IT), XF, XL, DX, R.
      IFLAG
      WRITE(6,500) (DELTAE(I), I=1, IDE), (TEE(I), I=1, IT), XF, XL, DX, R, FLAG
      DO 50 I=1, IT
      T=TEE(I)
      RT=T*R
      DO 49 J=1, IDE
      DELE=DELTAE(J)
      WRITE (6,200) T, DELE
      W=DELE/RT
      EXPW = EXP(W)
      EXPNW = EXP(-W)
      X=XF
      IF(FLAG.GT.0.) WRITE(6,300) RT, W, EXPW, EXPNW, X
10 CALL XSUBAB(X, EXPNW, XA, XB, FLAG, $11)
      CALL PRELIM(XA, XB, EXPNW, EXPW, SMALLR, S, FLAG)
      CALL DELGCX(DELE, RT, XA, XB, SMALLR, S, DLGCXS, FLAG)
      CALL DELGMX(X, XA, XB, R, DELE, DLGCXS, DGMEXS, FLAG)
      DELGXS=((XA*ALOG(XA)+XB*ALOG(XB)+(1.-XA)*ALOG(1.-XA)+(1.-XB)*ALOG(
11.-XB))*RT+XB*DELE)*(1.-X)/2.
      WRITE(6,400) X, DLGCXS, DGMEXS, DELGXS
      IF(FLAG.EQ.1.) FLAG=0.
11 X=X+DX
      IF(X.LE.XL) GO TO 10
49 CONTINUE
50 CONTINUE
100 FORMAT(2I2/(5E13.7 ))
200 FORMAT(1H139X4HT = E15.8,10X10HDELTA E = E15.8/1H038X1HX14X12HDELT
      1A G C XS 7X13HDELTA G ME XS 9X10HDELTA G XS/)
300 FORMAT(1H026X5E16.8)
400 FORMAT(27X4E20.8)
500 FORMAT(1H1/(26X5E16.8 ))
      GO TO 1
      END

```

```

$IBFTC XSBAB  FULIST
      SUBROUTINE XSUBAB(X,EXPW,XA,XB,FLAG,*)
      ASTAR=1.-EXPW
      CONJX=1.-X
      BSTAR=((1.+X)*EXPW-3.*X+1.)/CONJX
      CSTAR=-2.*X/CONJX*EXPW
      XB1=-BSTAR/2./ASTAR
      XB2=SQRT(BSTAR*BSTAR-4.*ASTAR*CSSTAR)/2./ASTAR
      XB=XB1+XB2
      IF((XB.GT.0.).AND.(XB.LT.1.))GO TO 10
      XB=XB1-XB2
      IF((XB.GT.0.).AND.(XB.LT.1.))GO TO 10
      WRITE (6,100)XB,ASTAR,BSTAR,CSSTAR
100  FORMAT(6H0XB = E15.8,38H , IS NOT IN THE RANGE (0 LT XB LT 1)./
      1 9H0ASTAR = E15.8,10X 8HBSTAR = E15.8,10X8HCSTAR = E15.8/
      216H0GO TO NEXT CASE)
      9 RETURN 1
10  XA=2./CONJX*X-XB
      IF((XA.GT.0.).AND.(XA.LT.1.))GO TO 12
      WRITE (6,200)XA,ASTAR,BSTAR,XB
200  FORMAT(6H0XA = E15.8,38H , IS NOT IN THE RANGE (0 LT XA LT 1)./
      1 9H0ASTAR = E15.8,10X 8HBSTAR = E15.8,10X 8HCSTAR = E15.8,10X
      25HXB = E15.8/16H0GO TO NEXT CASE)
      GO TO 9
12  IF(FLAG.LE.0.)GO TO 14
      WRITE (6,300)XA,XB,ASTAR,BSTAR,CSSTAR
300  FORMAT( 21H0D U M P  X S U B A B/6H0XA = E15.8,5X5HXB = E15.8,5X
      18HASTAR = E15.8,5X8HBSTAR = E15.8,5X,8HCSTAR = E15.8/)
14  RETURN
      END
$IBFTC PRLIM  FULIST
      SUBROUTINE PRELIM( XA,XB,EXPW,EXPW,SMALLR,S,FLAG)
      CONJXA=1.-XA
      CONJXB=1.-XB
      U=XA/CONJXA*EXPW
      V=XB/CONJXB*EXPW
      RNUM=((1.+U)*CONJXA)**2
      SMALLR=RNUM/(RNUM+EXPW)
      SNUM=((1.+V)*CONJXB)**2
      S=SNUM/(SNUM+EXPW)
      IF(FLAG.LE.0.)GO TO 1
      WRITE (6,100)U,V,RNUM,SMALLR,SNUM,S
100  FORMAT(21H0D U M P  P R E L I M/5H0U = E15.7,5H V = E15.7,8H RNUM
      1= E15.7, 9HSMALLR = E15.7,8H SNUM = E15.7,5H S = E15.7/)
1  RETURN
      FND

```

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R

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N
O
P

```

SIBFTC DGCSX FULIST
SUBROUTINE DELGCX (DELE,RT,XA,XB,SMALLR,S,DLGCXS,FLAG)
DLGCXS=(ALOG(XA/(1.-XA))*SMALLR + ALOG(XB/(1.-XB))*S)*RT + S*DELE
IF(FLAG.GT.0.)WRITE(6,100)DLGCXS
RETURN
100 FORMAT(21HOD U M P D L G C X S/13H0 DEL GCXS = E15.7/)
END

SIBFTC DGMX FULIST
SUBROUTINE DELGMX (X,XA,XB,RT,DELE,DLGCXS,DGMEXS,FLAG)
CONJXA=1.-XA
CONJXB=1.-XB
ZAMX=ALOG(CONJXA)*CONJXA + ALOG(XA)*XA
ZBMX=ALOG(CONJXB)*CONJXB + ALOG(XB)*XB
DGMEXS=((ZAMX+ZBMX)*RT+XB*DELE)/2.-X/(1.-X)*DLGCXS
IF(FLAG.GT.0.)WRITE (6,100)ZAMX,ZBMX,DGMEXS
RETURN
100 FORMAT(21HOD U M P D E L G M X/8H0ZAMX = E15.7,10X7HZBMX = E15.7,
110X9HDGMEXS = E15.7/)
END

SIBFTC DGMS FULIST
SUBROUTINE DGMES(X,RT,ALPHA,GME,DGMESG,GC,DELGF,FLAG)
IF(X=.5)10,20,30
10 DGMESG =ALOG((1.-2.*X)/(1.-X))*RT + 2.*DELGF + GC
GO TO 40
20 DGMESG = ALOG((1.-2.*ALPHA)/ALPHA)*RT - GME
GO TO 40
30 DGMESG = ALOG((1.-X)/(2.*X-1.))*RT - GME
40 IF(FLAG.GT.0.)WRITE(6,100) DGMESG
100 FORMAT(19HOD U M P D G M E S/10H0DGMESG = E15.8/)
RETURN
END

SIBFTC DGCS FULIST
SUBROUTINE DGCSIG(X,GC,GME,ALPHA,DELGF,RT,DLGCSG,FLAG)
IF(X=.5)10,20,30
10 DLGCSG = ALOG(X/(1.-2.*X))*RT -GC
GO TO 40
20 DLGCSG = ALOG((1.-2.*ALPHA)/ALPHA)*RT-GC
GO TO 40
30 DLGCSG = ALOG((2.*X-1.)/X)*RT + 2.*DELGF + GME
40 IF(FLAG.GT.0.)WRITE(6,100)DLGCSG
100 FORMAT(21HOD U M P D G C S I G/10H0DLGCSG = E15.7/)
RETURN
END

```

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APPENDIX II.

Computer program for calculating the excess free energies of the Me_2C phases in terms of $2 + w$ gramatom of alloy. For theoretical background of this problem, refer to AFML-TR-65-2, Part I, Volume I (1965).....(Bill Reuss).

```

SEXECUTE      IBJOB
$IBJOB 42051  MAP
$IBFTC 42051  FULIST,DECK,REF

```

```

C  PROGRAM C (42051)  ME2CY PHASE CALCULATION - EXCESS QUANTITIES
      DIMENSION Y(2500), XCA(2500), XCB(2500), ZA(2500), ZB(2500),
      1      Z(2500), HXS(2500), GXS(2500)

10  READ (5,20) MODEL, YMIN, YMAX, DY, WMIN, WMAX, DW
      FORMAT (11,8X,6E10,0)
      WRITE (6,30) MODEL,YMIN,YMAX,DY,WMIN,WMAX,DW
30  FORMAT(1H1//////////61X,9HPROGRAM C//62X,7H(42051)///44X,
      1 44HME2CY PHASE CALCULATIONS - EXCESS QUANTITIES///62X,6HMODEL ,
      2 11///3X,6HYMIN = F11.5 ,4X, 6HYMAX = F11.5 ,4X, 6H DY = F11.5,
      3 4X, 6HWMIN = F11.5,4X, 6HWMAX = F11.5 ,4X, 6H DW = F11.5 )

      W = WMIN

35  LINCT = 50
37  DO 39 I=1,2500
      Y(I) = 0.
      XCA(I) = 0.
      XCB(I) = 0.
      ZA(I) = 0.
      ZB(I) = 0.
      Z(I) = 0.
      HXS(I) = 0.
39  GXS(I) = 0.

40  I = 1
      Y(I) = YMIN
      EMW = 1./ EXP(W)

      50 GO TO (100,200),MODEL

100  AA = 2.* (1.-EMW)
      AAAA = 2. * AA
105  B = 1. - Y(I) + EMW*(1.+Y(I))
      C = Y(I) * EMW
      QUAD = B**2 + AAAA*C
      IF (QUAD) 107,110,110

107  ZA(I) = 1.
      ZP(I) = QUAD
      GO TO 280

110  QUAD = SQRT(QUAD)
      XCB(I) = (-B+QUAD)/AA
      IF (XCB(I)-1.)120,130,130
120  IF (XCB(I))130,130,160
130  ZB(I) = XCB(I)
      XCB(I) = (-B-QUAD)/AA
      IF (XCB(I)) 150,155,140
140  IF (XCB(I)-1.)160,150,150
150  Z(I) = XCB(I)
      XCB(I) = 0.
155  ZA(I) = 3.
      GO TO 280

160  XCA(I) = Y(I) - XCB(I)
      ZA(I) = XCA(I)* ALOG(XCA(I)) + (1.-XCA(I))*ALOG(1.-XCA(I))

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```

ZB(I)= XCB(I)*ALOG(XCB(I)) + (1.-XCB(I))* ALOG(1.-XCB(I))
HXS(I) = XCB(I) * W
GO TO 270

200 CON = -2. +4.* EMW
205 YEMW = Y(I) * EMW
A = CON + Y(I) - YEMW
B = 2. - YEMW
QUAD = B**2 + 4.*A*Y(I)
IF (QUAD) 107,210,210

210 QUAD = SQRT(QUAD)
AA = 2.*A
XCA(I) = (-B + QUAD)/AA
IF (XCA(I)-1.)220,230,230
220 IF (XCA(I)) 230,230,260
230 ZP(I) = XCA(I)
XCA(I) = (-B-QUAD)/AA
IF (XCA(I)) 250,255,240
240 IF (XCA(I) - 1.) 260,250,250
250 Z(I) = XCA(I)
255 ZA(I) = 2.
GO TO 280

260 XCA1 = 1. + XCA(I)
XCB(I) = Y(I)/2.*XCA1/XCA(I) - 1.
TO1PX = 2./XCA1
TXO1PX = TO1PX * XCA(I)
ZA(I)= TO1PX * ( XCA(I)*ALOG(XCA(I))+(1.-XCA(I))* ALOG(1.-XCA(I)))
ZB(I)=TXO1PX * ( XCB(I)*ALOG(XCB(I))+(1.-XCB(I))* ALOG(1.-XCB(I)))
HXS(I) = TXO1PX * XCB(I) * W

270 Z(I) = ZA(I) + ZP(I)
GXS(I) = HXS(I) + Z(I)
IF (I - 2499)280, 300 ,300

280 Y(I+1) = Y(I) + DY
IF (Y(I+1) - YMAX) 290,290,298
290 I = I+1
GO TO (105,205),MODEL

298 Y(I+1) = 0.
300 DO 380 J = 1,I
303 IF (LINCT - 42) 305,350,350
350 LINCT = 0
WRITE (6,360)MODEL ,W
360 FORMAT (1H1,61X, 9HPROGRAM C //62X, 7H(42051) ///44X,44HME2CY PHAS
1E CALCULATIONS - EXCESS QUANTITIES/// 62X , 6HMODEL ,11///
2 57X, 3HW = E15.8 ////)
305 IF (XCB(J)) 330,310,330
310 IF (ZA(J)- 1.) 320,315,320
315 WRITE (6,316) Y(J) ,ZB(J)
316 FORMAT(F11.4,21X,31HNEGATIVE VALUE UNDER RADICAL = E16.8,6X ,
1 15HIMAGINARY ROOTS )
GO TO 375
320 IF (ZA(J)-3.) 325,327,325
327 WRITE (6,328) Y(J) , ZP(J), Z(J)
328 FORMAT( F11.4,13X, 11HXC9 ROOTS ( ,E16.8 , 3H , ,E16.8 , 40H ) A
1RE NOT IN THE RANGE BETWEEN 0 AND 1 )

```

```

      GO TO 375
323 IF (ZA(J) - 2.) 330,323,330
323 WRITE (6,324) Y(J) , ZB(J) , Z(J)
324 FORMAT (F11.4,13X, 11HXCA ROOTS ( ,E16.8 , 3H , ,E16.8 , 40H ) A
      IRE NOT IN THE RANGE BETWEEN 0 AND 1 )
      GO TO 375
330 CALL INT4D (Y,HXS,Y(J) ,TRP, DHXS )
      CALL INT4D(Y,Z ,Y(J),TRP,DZ)
      CALL INT4D(Y,GXS,Y(J),TRP,DGXS)
370 WRITE (6,371) Y(J) ,XCA(J) , XCB(J) ,ZA(J),ZB(J),Z(J) ,HXS(J),
      1 GXS(J), DHXS , DZ , DGXS
371 FORMAT (1X,4HY = E15.8,8H XCA = E15.8,8H XCB = E15.8,7H ZA =
      1 E15.8,7H ZB = E15.8,6H Z = E15.8/5X,6HHXS = E15.8,8H GXS =
      2 E15.8,12H DHXS/DY = E15.8,10H DZ/DY = E15.8,12H DGXS/DY =
      3 E15.8)
375 LINCT = LINCT + 2
380 CONTINUE

```

```

      W = W+DW
      IF (W-WMAX) 35,35,10

```

END

SENTRY 42051

\$DATA

1	.96	1.04	.02	.68315768	.70315768	.01
2	.96	1.04	.02	.68315768	.70315768	.01
2	.05	1.95	.05	.5	9.	.5
1	.05	1.95	.05	.5	9.	.5

APPENDIX III.

Computer program for evaluating the high-temperature thermodynamic properties. For theoretical background, refer to AFML-TR-65-2, Part IV, Volume I (1965)..... (Len Nole).

```

$IBJOB          GO,MAP
$IBFTC 8064     LIST,REF,DECK
C      EVALUATION OF HIGH TEMPERATURE THERMODYNAMIC PROPERTIES
C      VIA NUMERICAL INTEGRATION
      DIMENSION DATA(500),HEAD(12),TABLT(100),KDIS(20),TABLY(100),
1      TABT(1),TABY(1)
      EQUIVALENCE (TABT,DATA(1)),(TABY,DATA(201)),(SST,DATA(401))
C
C
1 DO 2 I =1,500
2 DATA(I) = 0.
  CALL SLITE(0)
  CALL AS138 (DATA,HEAD,NE)
  IF (NE - 2)6,3,4
3 STOP
4 WRITE (6,5)
5 FORMAT (27H (((I N P U T   E R R O R))))
  GO TO 1
6 N = DATA(402)
  DO 10 I =1,200
  IF (TABT(I))4,7,10
  7 IF (TABT(I+1))4,11,10
10 CONTINUE
11 NOFT = I-1
  WRITE (6,12) HEAD
12 FORMAT (1H1,42X,27HAEROJAY GENERAL CORPORATION/ 36X,41H LIQUID ROCK
1ET PLANT,SACRAMENTO CALIFORNIA / 31X,55HEVALUATION OF HIGH TEMPERA
2TURE THERMODYNAMIC PROPERTIES/11H DEPT. 4600,80X,8HJOB-8064/32X,
312A6)
  WRITE (6,13) SST, N, (TABT(I),TABY(I),TABT(I+50),TABY(I+50),
1TABT(I+100),TABY(I+100),TABT(I+150),TABY(I+150), I = 1,50)
13 FORMAT (///,50X,20H I N P U T   D A T A   ///,7X,9HSST,3X,7HSUB INT/,
1F10.2,8X,12,///,23X,2HT ,8X,2HY ,10X,10H      T(50),10H      Y(50),10
2X,10H      T(100),10H      Y(100),10X,10H      T(150),10H      Y(150),//,
3(15X,F10.2,F10.3,10X,F10.2,F10.3,10X,F10.2,F10.3,10X,F10.2,F10.3))
  WRITE (6,130)
130 FORMAT (1H1,48X,21H O U T P U T   D A T A   //,10H T DEG K ,5X,
15H Y ,5X,5H CP ,4X,6HHT-HST,4X,6HST-SST,5X,5HFOGFE,5X,10H INTER
2VALS)
  KDIS(1) = 1
  I = 2
  K = 2
  TINTP = 0.
  TABLT(1) = TABT(1)
  TABLY(1) = TABY(1)
  J = 2
14 TABLT(I) = TABT(J)
  TABLY(I) = TABY(J)
  IF (TABT(J+1))20,16,20
16 IF (TABT(J+2))4,22,160
160 J = J+2
  I = I+1
  KDIS(K) = J
  K = K + 1
  TABLT(I) = TABT(J)
  TABLY(I) = TABY(J)
20 I = I + 1
  J = J+4
  GO TO 14

```

```

22 KDIS(K) = NOFT
   K = 0
   LMN = 1
24 K = K+1
   NML = KDIS(K)
   LN = KDIS(K+1)
   IF (LMN - 1) 231, 231, 25
231 DELHT = 0.
   DELST = 0.
   CP = TABLY(1)
   FOGFE = DATA(401)
   GO TO 27
25 LMN = LMN+1
   DELHT = TABLY(LMN)*(TABLT(LMN) - 298.15)
   CALL INT4D (TABT(NML), TABY(NML), TABLT(LMN), YO, DY)
   CP = DY*(TABLT(LMN) - 298.15) + TABLY(LMN)
   TEMP = TABLY(LMN)*(1. - 298.15/TABLT(LMN))
   CALL SLITET(1, KL)
   IF (KL - 1) 26, 26, 251
251 CALL INTGR (TABLT(LMN-1), TABLT(LMN), TX, N)
   CALL INT4 (TABT(NML), TABY(NML), TX, YOFT)
   GOFTX = YOFT * (TX - 298.15)/TX/TX
   CALL INTGS (GOFTX, TINT, .00001, M)
   TINT = TINT + TINTP
   TINTP = TINT
26 DELST = TEMP + TINT
   FOGFE = -DELHT/TABLT(LMN) + DELST + SST
27 WRITE (6, 30) TABLT(LMN), TABLY(LMN), CP, DELHT, DELST, FOGFE, M
30 FORMAT (F10.2, F10.3, 4F10.2, 12X, I3)
31 IF (TABLT(LMN)) 4, 1, 32
32 IF (TABLT(LMN) - TABT(LN)) 25, 34, 34
34 IF (TABT(LN) - TABT(NOFT)) 35, 1, 1
35 CALL SLITE(1)
   GO TO 24
END
SENTRY      8064
$DATA

```

APPENDIX IV.

Computer program for calculating the free energies of the monocarbide phases using the Wagner-Schottky vacancy model. For theoretical background, refer to AFM^U-TR-65-2, Part IV, Volume I (1965).....(Jerry Howard)

```

$EXECUTE      IPJOB
$IBJOB 8072   MAP
$IAFTC 8072   LIST,DECK

```

C
C

MONOCARBIDES BY USING THE VACANCY MODEL.

C8072- PROGRAM H. THERMODYNAMIC CALCULATIONS FOR GROUP IV METAL

DIMENSION DATA(200),HEAD(12),TEMP1(20),GAO(20),GB0(20),

1 ALGPA0(20),ALGPB0(20),GA(20),GB(20),RTLN(20),

2 ALFA(20),TDGF(20)

DIMENSION A(20),B(20),BET(20),GAM(20)

EQUIVALENCE (DATA(1),TA),(DATA(2),TAB),(DATA(3),TEL),(DATA(4),

1 BETA),(DATA(5),GAMMA),(DATA(6),BETAP),(DATA(7),GAMMAP),

2 (DATA(8),BETAPP),(DATA(9),GAMMPP),(DATA(11

3),XMIN),(DATA(12),XMAX),(DATA(13),DELX),

4 (DATA(15),TFMP1),(DATA(55),GAO),

5 (DATA(75),GB0),(DATA(95),ALGPA0),(DATA(115),ALGPB0),

6 (DATA(155),T1CONT),(DATA(35),AA),(DATA(36),BB),(DATA(37)

7 ,AAP),(DATA(38),BPP),(DATA(39),AAPP),(DATA(40),BPPP)

C

1 CALL AS138(DATA,HEAD,NE)

WRITE(6,88)

88 FORMAT(1H1)

GO TO (5,4,2),NE

2 WRITE(6,3)

3 FORMAT(20X,24H I N P U T E R R O R)

GO TO 1

4 CALL EXIT

5 PT5=.005

ALN2=.69315

R=1.98726

I=1

ICNT1=T1CONT+ .01

C

6 T = TEMP1(I)

IF(T.LT.TAE) GO TO 7

IF(T.LT.TBL) GO TO 8

BET(I)=BETAPP

GAM(I)=GAMMPP

A(I) = AAP

B(I) = BPP

GO TO 9

7 BET(I)=BETA

GAM(I)=GAMMA

A(I) = AA

B(I) = BB

GO TO 9

```

8 BET(I)=BETAP
  GAM(I)=GAMMAP
  A(I) = AAP
  B(I) = BRP
9 RT=R*T
  TDGF(I)=BET(I)+GAM(I)*T
  GB(I)=A(I)+B(I)*T
  RTLN(I)=-GB(I)-RT*ALN2
  ALFA(I)=.5*EXP(-GB(I)/RT)
  GA(I)=-RTLN(I)-RT*ALN2-TDGF(I)
C
  I=I+1
  IF(I.LE.ICNT1) GO TO 6
C
20 J=1
C
21 T=TEMP1(J)
  CGA = GA(J)
  CGB = GB(J)
  CRLNA = RTLN(J)
  CALF = ALFA(J)
  RT = R*T
  WRITE(6,22) HEAD
22 FORMAT(1H1,42X,27HAEROJET GENERAL CORPORATION/36X,41H LIQUID ROCKET
  1 PLANT,SACRAMENTO CALIFORNIA//38X,12A6//19H I N P U T D A T A//)
  WRITE(6,100) BET(J),GAM(J), A(J), B(J)
100 FORMAT(9X,16H LINEAR EQUATIONS/12X,18H2 DELTA GF      A = ,E12.5,
  16H, B = ,E12.5/12X,18HGB+      A = ,E12.5,6H, B = ,E12.5)
  WRITE(6,101)GAO(J),GBO(J),ALGPAO(J),ALGPBO(J)
101 FORMAT(9X,6HGAO = ,F7.0,8H, GBO = ,F7.0,12H, LOG PAO = ,F7.3,
  112H, LOG PRO = ,F7.3)
28 WRITE(6,29) T
29 FORMAT(9X,15H TEMPERATURE IS ,F6.1,15H DEGREES KELVIN,/)
  WRITE(6,102) CGA,CGB,CRLNA,CALF
102 FORMAT(21H O U T P U T D A T A//9X,5HGA+= ,E12.5,6H,GB+= ,E12.5,
  113H,RT LN ALFA= ,E12.5,7H,ALFA= ,E12.5//8X,1HX,11X,4H DGAB,10X,
  24H DGGB,11X,2H DG,12X,3H GAB,11X,3H GBB,12X,1HG,10X,6H LOG PA,8X,
  36H LOG PB)
  C1=4.576*T
  C2=C1*ALGPAO(J)
  C3=C1*ALGPBO(J)
  X=XMIN
C
30 ARG = ABS(X/.5-1.0)
  IF(ARG.LE.1.E-4) GO TO 32
  IF(X.LT.0.5) GO TO 34

```

```

      IF(X.GT.0.5) GO TO 35
32  X = .500
      DGA = -CGA-RT*ALN2-CRLNA
      DGB = -CGB+CGA+DGA
      GO TO 36
34  DGA = TDGF(J)+CGB+RT*ALOG((1.-2.*X)/(1.-X))
      DGB = -CGB+RT*ALOG(X/(1.-2.*X))
      GO TO 36
35  DGA = -CGA+RT*ALOG((1.-X)/(2.*X-1.))
      DGB = TDGF(J)+CGA+RT*ALOG((2.*X-1.)/X)
36  VR1 = 1. -X
      DG=VR1*DGA+DGB*X
      GAB=DGA+GAO(J)
      GBR=DGR+GBO(J)
      G=VR1*GAB+X*GBR
      ALGPA=(DGA+C2)/C1
      ALGPB=(DGR+C3)/C1
      WRITE(6,33) X,DGA,DGR,DG,GAB,GBR,G,ALGPA,ALGPB
33  FORMAT(9(2X,F12.5))
      X=X+DELX
      IF(X.LE.XMAX) GO TO 30
      J=J+1
      IF(J.LE.ICNT1) GO TO 21
      GO TO 1
      END

```

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<p>The general conditional equations which govern the phase equilibria in three-component systems are presented. Using the general conditional equations, a general method has been developed to precalculate the phase equilibria in three-component systems from first principle using computer technique. The method developed has been applied to several model examples and the system Ta-Hf-C. The phase equilibria in three-component systems calculated using the simplified method as originally developed by Rudy, agree well with those calculated by the present method. The only difference is in the homogeneous range with respect to the interstitial component of solid solutions which exhibit large variation with metal exchange. This is to be expected in view of the assumptions made in the simplified method.</p> <p>In connection with the phase diagram calculation and other problems of the present Air Force contract, several computer programs have been developed which are included in the appendix of this report.</p>	

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